KinomeX: a web application for predicting kinome-wide polypharmacology effect of small molecules

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# 1 Methods

## 1.1 The scheme of model building and evaluation



### Supplementary figure 1. The scheme of model building and evaluation.

## 1.2 Definitions of sub-family selectivity

We defined the odds ratio (OR) as a measure of group-specific selectivity (Bland, et al., 2000). For example, to calculate the strength of the association between an inhibitor for the group of TK, the OR statistic can be calculated as:

OR = (NTP/NOP)/(NTN/NON) ,

where NTP refers to the number of positive interactions of the inhibitor within the TK family and NOP refers to the number of its positive interactions with kinases other than TK. Similarly, NTN and NON are defined as the number of negative interactions for TK and other kinases, respectively. If the OR is significantly greater than 1.0, the kinases inhibited by this inhibitor can be considered to be enriched in the TK group, indicating that the inhibitor is TK-selective

# 2 Datasets

## 2.1 Modelling dataset

We merged Kinase SARfari database version 6.00 (https://chembl.gitbook.io/chembl-interface-documentation/legacy-resources#kinase-sarfari) and the Metz dataset (Metz, et al., 2011) to generate the model. The inhibition activity in the merged dataset was converted to two classes: active (pKi/pKd/pIC50 ≥ 6) and inactive (pKi/pKd/pIC50＜6). After the deletion of mutant kinases and kinases without both active and inactive data points, the final dataset contains over 170,000 bioactivity data points composed of 391 kinases (Supplementary table 1) and ~32,000 compounds. The dataset is divided into 80% training and 20% testing datasets by random selection of compounds. The information of kinases and numbers of positive and negative samples for each kinase in modelling dataset are shown in supplementary table 1, and the exact modelling dataset can be downloaded from <https://kinome.dddc.ac.cn/en/page/about/>.

### Supplementary table 1. The information of predictable kinases.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| UniProt ID | Name | Classification | Organism | number of positive samples | number of negative samples |
| Q9HAZ1 | hCLK4 | CMGC | Homo sapiens | 568 | 519 |
| P49760 | hCLK2 | CMGC | Homo sapiens | 259 | 693 |
| P36894 | hBMPR1A | TKL | Homo sapiens | 7 | 34 |
| Q59H18 | hTNNI3K | TKL | Homo sapiens | 1 | 40 |
| P80192 | hMAP3K9 | TKL | Homo sapiens | 36 | 47 |
| Q9UQ88 | hPITSLREb | CMGC | Homo sapiens | 4 | 36 |
| Q9Y4K4 | hMAP4K5 | STE | Homo sapiens | 247 | 451 |
| O00506 | hSTK25 | STE | Homo sapiens | 5 | 36 |
| Q14164 | hIKBKE | Other | Homo sapiens | 52 | 323 |
| P27361 | hERK1 | CMGC | Homo sapiens | 105 | 354 |
| Q96RR4 | hCAMKK2 | Other | Homo sapiens | 17 | 51 |
| Q9H1R3 | hMYLK2 | CAMK | Homo sapiens | 10 | 32 |
| P26618 | mPDGFRa | TK | Mus musculus | 28 | 94 |
| P15056 | hBRAF | TKL | Homo sapiens | 345 | 177 |
| Q9UKE5 | hTNIK | STE | Homo sapiens | 11 | 32 |
| Q13470 | hTNK1 | TK | Homo sapiens | 11 | 31 |
| Q13627 | hDYRK1A | CMGC | Homo sapiens | 337 | 807 |
| P42679 | hMATK | TK | Homo sapiens | 31 | 432 |
| P11799 | gMYLK | CAMK | Gallus gallus | 35 | 97 |
| P57059 | hSNF1LK | CAMK | Homo sapiens | 6 | 36 |
| O14733 | hMKK7 | STE | Homo sapiens | 1 | 3 |
| Q96L34 | hMARK4 | CAMK | Homo sapiens | 17 | 44 |
| Q9H3Y6 | hSRMS | TK | Homo sapiens | 46 | 453 |
| Q9Y616 | hIRAK3 | TKL | Homo sapiens | 5 | 36 |
| Q9BYT3 | hSTK33 | CAMK | Homo sapiens | 6 | 43 |
| P50613 | hCDK7 | CMGC | Homo sapiens | 129 | 358 |
| O15530 | hPDPK1 | AGC | Homo sapiens | 215 | 731 |
| O95747 | hOXSR1 | STE | Homo sapiens | 1 | 5 |
| Q13882 | hPTK6 | TK | Homo sapiens | 42 | 401 |
| Q13554 | hCAMK2B | CAMK | Homo sapiens | 60 | 673 |
| Q9WUI1 | mMAPK11 | CMGC | Mus musculus | 33 | 1 |
| P22694 | hPKAb | AGC | Homo sapiens | 65 | 474 |
| P00516 | bPRKG1 | AGC | Bos taurus | 11 | 13 |
| O94804 | hSTK10 | STE | Homo sapiens | 18 | 25 |
| O14757 | hChk1 | CAMK | Homo sapiens | 1096 | 1252 |
| O75385 | hULK1 | Other | Homo sapiens | 2 | 5 |
| P04409 | bPKCa | AGC | Bos taurus | 4 | 1 |
| P52333 | hJAK3 | TK | Homo sapiens | 162 | 727 |
| P70618 | rp38a | CMGC | Rattus norvegicus | 44 | 8 |
| P05771 | hPKCb1 | AGC | Homo sapiens | 267 | 467 |
| O75914 | hPAK3 | STE | Homo sapiens | 5 | 56 |
| P35916 | hVEGFR3 | TK | Homo sapiens | 284 | 622 |
| P49840 | hGSK3a | CMGC | Homo sapiens | 522 | 987 |
| Q92918 | hMAP4K1 | STE | Homo sapiens | 13 | 29 |
| P48730 | hCSNK1D | CK1 | Homo sapiens | 168 | 643 |
| Q9H2X6 | hHIPK2 | CMGC | Homo sapiens | 207 | 484 |
| Q8NFD2 | hANKK1 | TKL | Homo sapiens | 8 | 33 |
| P42681 | hTXK | TK | Homo sapiens | 15 | 39 |
| P08631 | hHCK | TK | Homo sapiens | 194 | 170 |
| P53350 | hPLK1 | Other | Homo sapiens | 300 | 975 |
| P53779 | hJNK3 | CMGC | Homo sapiens | 350 | 390 |
| Q64725 | rSYK | TK | Rattus norvegicus | 2 | 1 |
| Q6DT37 | hCDC42BPG | AGC | Homo sapiens | 3 | 37 |
| P36896 | hALK4 | TKL | Homo sapiens | 5 | 36 |
| Q9BXA7 | hTSSK1 | CAMK | Homo sapiens | 53 | 496 |
| Q9JI10 | mSTK3 | STE | Mus musculus | 4 | 1 |
| Q92772 | hCDKL2 | CMGC | Homo sapiens | 2 | 5 |
| Q06187 | hBTK | TK | Homo sapiens | 106 | 680 |
| Q9NR20 | hDYRK4 | CMGC | Homo sapiens | 32 | 510 |
| Q9Y6E0 | hSTK24 | STE | Homo sapiens | 7 | 35 |
| P16234 | hPDGFRa | TK | Homo sapiens | 310 | 460 |
| Q96SB4 | hSRPK1 | CMGC | Homo sapiens | 46 | 598 |
| P05480 | mSRC | TK | Mus musculus | 18 | 11 |
| Q8TDX7 | hNEK7 | Other | Homo sapiens | 1 | 41 |
| O75676 | hMSK2 | AGC | Homo sapiens | 16 | 16 |
| Q8TD08 | hERK7 | CMGC | Homo sapiens | 10 | 33 |
| Q13043 | hSTK4 | STE | Homo sapiens | 15 | 41 |
| Q15831 | hSTK11 | CAMK | Homo sapiens | 6 | 37 |
| Q13131 | hPRKAA1 | CAMK | Homo sapiens | 164 | 754 |
| P19525 | hEIF2AK2 | Other | Homo sapiens | 4 | 39 |
| O14920 | hIKBKB | Other | Homo sapiens | 419 | 580 |
| Q96PY6 | hNEK1 | Other | Homo sapiens | 2 | 42 |
| Q8MMZ8 | eimPKG | AGC | Eimeria tenella | 254 | 3 |
| P51817 | hPRKX | AGC | Homo sapiens | 202 | 586 |
| Q9UHD2 | hTBK1 | Other | Homo sapiens | 44 | 285 |
| Q13237 | hPRKG2 | AGC | Homo sapiens | 80 | 484 |
| P22455 | hFGFR4 | TK | Homo sapiens | 26 | 99 |
| Q02750 | hMEK1 | STE | Homo sapiens | 397 | 449 |
| Q8N5S9 | hCAMKK1 | Other | Homo sapiens | 9 | 33 |
| Q9UPE1 | hMSSK1 | CMGC | Homo sapiens | 3 | 5 |
| P05131 | bPKAb | AGC | Bos taurus | 11 | 80 |
| P36888 | hFLT3 | TK | Homo sapiens | 648 | 796 |
| P20786 | rPDGFRa | TK | Rattus norvegicus | 24 | 19 |
| Q9H4B4 | hPLK3 | Other | Homo sapiens | 81 | 644 |
| P04629 | hNTRK1 | TK | Homo sapiens | 270 | 821 |
| O43283 | hMAP3K13 | TKL | Homo sapiens | 3 | 4 |
| Q9UPZ9 | hICK | CMGC | Homo sapiens | 2 | 6 |
| Q8IVH8 | hMAP4K3 | STE | Homo sapiens | 12 | 30 |
| P30530 | hAXL | TK | Homo sapiens | 167 | 312 |
| Q13555 | hCAMK2G | CAMK | Homo sapiens | 94 | 616 |
| P33981 | hMPS1 | Other | Homo sapiens | 9 | 37 |
| Q86Z02 | hHIPK1 | CMGC | Homo sapiens | 1 | 10 |
| Q9BWU1 | hCDC2L6 | CMGC | Homo sapiens | 21 | 216 |
| O14578 | hCIT | AGC | Homo sapiens | 11 | 31 |
| P11802 | hCDK4 | CMGC | Homo sapiens | 597 | 611 |
| P07949 | hRET | TK | Homo sapiens | 320 | 575 |
| Q9WUD9 | rSRC | TK | Rattus norvegicus | 23 | 15 |
| Q9C098 | hDCAMKL3 | CAMK | Homo sapiens | 4 | 37 |
| P21802 | hFGFR2 | TK | Homo sapiens | 62 | 103 |
| P09215 | rPKCd | AGC | Rattus norvegicus | 66 | 56 |
| Q96NX5 | hCAMK1G | CAMK | Homo sapiens | 3 | 37 |
| P63086 | rERK2 | CMGC | Rattus norvegicus | 1 | 14 |
| Q5S007 | hLRRK2 | TKL | Homo sapiens | 120 | 219 |
| O60674 | hJAK2 | TK | Homo sapiens | 173 | 661 |
| Q00537 | hPCTK2 | CMGC | Homo sapiens | 7 | 35 |
| Q8IW41 | hMAPKAPK5 | CAMK | Homo sapiens | 36 | 532 |
| Q16620 | hNTRK2 | TK | Homo sapiens | 171 | 783 |
| P49759 | hCLK1 | CMGC | Homo sapiens | 43 | 48 |
| P06493 | hCDK1 | CMGC | Homo sapiens | 837 | 1672 |
| P16591 | hFER | TK | Homo sapiens | 121 | 377 |
| P23443 | hRPS6KB1 | AGC | Homo sapiens | 279 | 548 |
| Q9H422 | hHIPK3 | CMGC | Homo sapiens | 4 | 4 |
| P49674 | hCSNK1E | CK1 | Homo sapiens | 16 | 49 |
| P27037 | hACVR2A | TKL | Homo sapiens | 1 | 39 |
| Q9UIK4 | hDAPK2 | CAMK | Homo sapiens | 5 | 41 |
| Q16513 | hPKN2 | AGC | Homo sapiens | 184 | 561 |
| Q02779 | hMAP3K10 | TKL | Homo sapiens | 23 | 54 |
| P78368 | hCSNK1G2 | CK1 | Homo sapiens | 92 | 556 |
| Q13546 | hRIPK1 | TKL | Homo sapiens | 7 | 36 |
| O43293 | hDAPK3 | CAMK | Homo sapiens | 263 | 711 |
| XP\_341554.1 | rPKCt | AGC | Rattus norvegicus | 66 | 56 |
| Q9UQM7 | hCAMK2A | CAMK | Homo sapiens | 63 | 400 |
| P41743 | hPKCi | AGC | Homo sapiens | 103 | 774 |
| Q13705 | hACVR2B | TKL | Homo sapiens | 2 | 41 |
| Q05655 | hPKCd | AGC | Homo sapiens | 92 | 652 |
| Q15139 | hPKD1 | CAMK | Homo sapiens | 97 | 320 |
| Q8IVW4 | hCDKL3 | CMGC | Homo sapiens | 2 | 4 |
| Q15303 | hHER4 | TK | Homo sapiens | 81 | 643 |
| Q16566 | hCAMK4 | CAMK | Homo sapiens | 6 | 63 |
| P06239 | hLCK | TK | Homo sapiens | 1192 | 1490 |
| P54753 | hEPHB3 | TK | Homo sapiens | 15 | 63 |
| P51451 | hBLK | TK | Homo sapiens | 208 | 422 |
| O15264 | hp38d | CMGC | Homo sapiens | 240 | 840 |
| P63319 | rPKCg | AGC | Rattus norvegicus | 116 | 116 |
| Q00534 | hCDK6 | CMGC | Homo sapiens | 5 | 42 |
| O76039 | hCDKL5 | CMGC | Homo sapiens | 1 | 5 |
| P08922 | hROS1 | TK | Homo sapiens | 113 | 378 |
| O00141 | hSGK | AGC | Homo sapiens | 107 | 733 |
| O94768 | hSTK17B | CAMK | Homo sapiens | 6 | 36 |
| P22612 | hPKAg | AGC | Homo sapiens | 60 | 442 |
| Q15569 | hTESK1 | TKL | Homo sapiens | 3 | 38 |
| P21709 | hEPHA1 | TK | Homo sapiens | 9 | 36 |
| Q9P289 | hMST4 | STE | Homo sapiens | 6 | 45 |
| Q15835 | hGRK1 | AGC | Homo sapiens | 4 | 4 |
| Q06418 | hTYRO3 | TK | Homo sapiens | 100 | 681 |
| Q9UKI8 | hTLK1 | Other | Homo sapiens | 4 | 36 |
| Q7KZI7 | hMARK2 | CAMK | Homo sapiens | 109 | 572 |
| Q16644 | hMAPKAPK3 | CAMK | Homo sapiens | 10 | 738 |
| P00533 | hEGFR | TK | Homo sapiens | 1789 | 2248 |
| O75116 | hROCK2 | AGC | Homo sapiens | 686 | 651 |
| P34947 | hGRK5 | AGC | Homo sapiens | 40 | 310 |
| P07333 | hCSF1R | TK | Homo sapiens | 628 | 804 |
| Q00536 | hPCTK1 | CMGC | Homo sapiens | 12 | 31 |
| P11362 | hFGFR1 | TK | Homo sapiens | 476 | 1307 |
| Q9Y5S2 | hCDC42BPB | AGC | Homo sapiens | 3 | 39 |
| Q99640 | hPKMYT1 | Other | Homo sapiens | 1 | 41 |
| P00517 | bPKAa | AGC | Bos taurus | 26 | 91 |
| Q9HC98 | hNEK6 | Other | Homo sapiens | 2 | 54 |
| Q9Y463 | hDYRK1B | CMGC | Homo sapiens | 127 | 286 |
| P54762 | hEPHB1 | TK | Homo sapiens | 8 | 35 |
| Q16816 | hPHKG1 | CAMK | Homo sapiens | 43 | 57 |
| P09619 | hPDGFRb | TK | Homo sapiens | 502 | 804 |
| P08069 | hIGF1R | TK | Homo sapiens | 581 | 1100 |
| P15735 | hPHKG2 | CAMK | Homo sapiens | 91 | 580 |
| Q9UEW8 | hSTK39 | STE | Homo sapiens | 2 | 5 |
| P06241 | hFYN | TK | Homo sapiens | 216 | 382 |
| Q9NYL2 | hZAK | TKL | Homo sapiens | 53 | 606 |
| P24941 | hCDK2 | CMGC | Homo sapiens | 1712 | 1748 |
| P41240 | hCSK | TK | Homo sapiens | 13 | 72 |
| Q96Q40 | hALS2CR7 | CMGC | Homo sapiens | 1 | 6 |
| O75716 | hSTK16 | Other | Homo sapiens | 11 | 34 |
| Q9P0L2 | hMARK1 | CAMK | Homo sapiens | 5 | 39 |
| Q04771 | hALK2 | TKL | Homo sapiens | 72 | 293 |
| Q04912 | hMST1R | TK | Homo sapiens | 108 | 256 |
| Q8TDC3 | hBRSK1 | CAMK | Homo sapiens | 62 | 580 |
| P00523 | gSRC | TK | Gallus gallus | 142 | 84 |
| P11309 | hPIM1 | CAMK | Homo sapiens | 397 | 1100 |
| Q9Y2H1 | hSTK38L | AGC | Homo sapiens | 3 | 39 |
| Q13976 | hPRKG1 | AGC | Homo sapiens | 118 | 453 |
| Q9NZJ5 | hPEK | Other | Homo sapiens | 18 | 18 |
| P32298 | hGRK4 | AGC | Homo sapiens | 4 | 4 |
| P0C264 | hSgK110 | Other | Homo sapiens | 1 | 6 |
| Q6PHR2 | hULK3 | Other | Homo sapiens | 2 | 5 |
| Q9H2K8 | hTAOK3 | STE | Homo sapiens | 3 | 5 |
| Q9UQB9 | hAURc | Other | Homo sapiens | 33 | 41 |
| P14616 | hINSRR | TK | Homo sapiens | 4 | 39 |
| P49187 | rJNK3 | CMGC | Rattus norvegicus | 36 | 39 |
| Q6P3R8 | hNEK5 | Other | Homo sapiens | 1 | 38 |
| P68400 | hCSNK2A1 | CMGC | Homo sapiens | 166 | 796 |
| P04626 | hHER2 | TK | Homo sapiens | 759 | 1074 |
| O00444 | hPLK4 | Other | Homo sapiens | 211 | 539 |
| P47811 | mp38a | CMGC | Mus musculus | 185 | 43 |
| P31749 | hAKT1 | AGC | Homo sapiens | 773 | 1151 |
| P36507 | hMEK2 | STE | Homo sapiens | 64 | 299 |
| Q01279 | mEGFR | TK | Mus musculus | 12 | 55 |
| P51617 | hIRAK1 | TKL | Homo sapiens | 87 | 516 |
| P50750 | hCDK9 | CMGC | Homo sapiens | 177 | 322 |
| Q8NEV4 | hMYO3A | STE | Homo sapiens | 3 | 38 |
| Q08881 | hITK | TK | Homo sapiens | 453 | 668 |
| O15111 | hCHUK | Other | Homo sapiens | 114 | 507 |
| Q92630 | hDYRK2 | CMGC | Homo sapiens | 3 | 6 |
| Q9H2G2 | hSLK | STE | Homo sapiens | 173 | 474 |
| P00519 | hABL1 | TK | Homo sapiens | 739 | 686 |
| P04049 | hRAF1 | TKL | Homo sapiens | 256 | 155 |
| Q13557 | hCAMK2D | CAMK | Homo sapiens | 85 | 546 |
| P30291 | hWEE1 | Other | Homo sapiens | 238 | 117 |
| Q8IYT8 | hULK2 | Other | Homo sapiens | 2 | 5 |
| Q2M2I8 | hAAK1 | Other | Homo sapiens | 12 | 31 |
| P05129 | hPKCg | AGC | Homo sapiens | 241 | 1099 |
| P42684 | hABL2 | TK | Homo sapiens | 70 | 108 |
| P12931 | hSRC | TK | Homo sapiens | 1470 | 1848 |
| P29320 | hEPHA3 | TK | Homo sapiens | 12 | 41 |
| Q9Y2K2 | hQSK | CAMK | Homo sapiens | 3 | 3 |
| O96017 | hChk2 | CAMK | Homo sapiens | 264 | 625 |
| XP\_620754.3 | mULK3 | Other | Mus musculus | 4 | 2 |
| O96013 | hPAK4 | STE | Homo sapiens | 110 | 984 |
| P53671 | hLIMK2 | TKL | Homo sapiens | 43 | 44 |
| Q8NE63 | hHIPK4 | CMGC | Homo sapiens | 157 | 458 |
| P68403 | rPKCb1 | AGC | Rattus norvegicus | 88 | 56 |
| P54760 | hEPHB4 | TK | Homo sapiens | 196 | 270 |
| Q86V86 | hPIM3 | CAMK | Homo sapiens | 107 | 540 |
| P48729 | hCSNK1A1 | CK1 | Homo sapiens | 131 | 841 |
| P53778 | hp38g | CMGC | Homo sapiens | 250 | 862 |
| Q96GD4 | hAURb | Other | Homo sapiens | 767 | 864 |
| P05132 | mPKAa | AGC | Mus musculus | 1 | 7 |
| P06240 | mLCK | TK | Mus musculus | 42 | 54 |
| P00520 | mABL1 | TK | Mus musculus | 8 | 4 |
| Q8N4C8 | hMINK1 | STE | Homo sapiens | 169 | 491 |
| Q16539 | hp38a | CMGC | Homo sapiens | 2196 | 1120 |
| P29317 | hEPHA2 | TK | Homo sapiens | 107 | 645 |
| Q9BZL6 | hPKD2 | CAMK | Homo sapiens | 131 | 637 |
| Q9NSY1 | hBMP2K | Other | Homo sapiens | 10 | 32 |
| Q8WTQ7 | hGRK7 | AGC | Homo sapiens | 5 | 3 |
| Q61851 | mFGFR3 | TK | Mus musculus | 11 | 18 |
| Q16659 | hERK3 | CMGC | Homo sapiens | 2 | 40 |
| P19784 | hCSNK2A2 | CMGC | Homo sapiens | 25 | 168 |
| Q8IY84 | hNIM1 | CAMK | Homo sapiens | 1 | 11 |
| Q8WXR4 | hMYO3B | STE | Homo sapiens | 3 | 38 |
| Q00526 | hCDK3 | CMGC | Homo sapiens | 7 | 75 |
| Q9UEE5 | hSTK17A | CAMK | Homo sapiens | 193 | 407 |
| Q9P286 | hPAK7 | STE | Homo sapiens | 5 | 37 |
| P70336 | rROCK2 | AGC | Rattus norvegicus | 1 | 2 |
| P43405 | hSYK | TK | Homo sapiens | 270 | 600 |
| P35968 | hVEGFR2 | TK | Homo sapiens | 2619 | 2223 |
| P35969 | mVGFR1 | TK | Mus musculus | 15 | 57 |
| Q9UBS0 | hRPS6KB2 | AGC | Homo sapiens | 14 | 15 |
| P31751 | hAKT2 | AGC | Homo sapiens | 324 | 871 |
| P49336 | hCDK8 | CMGC | Homo sapiens | 138 | 304 |
| O00238 | hBMPR1B | TKL | Homo sapiens | 1 | 5 |
| Q99759 | hMAP3K3 | STE | Homo sapiens | 3 | 5 |
| Q12851 | hMAP4K2 | STE | Homo sapiens | 249 | 650 |
| O60285 | hNUAK1 | CAMK | Homo sapiens | 9 | 54 |
| Q96RG2 | hPASK | CAMK | Homo sapiens | 16 | 64 |
| P11440 | mCDC2 | CMGC | Mus musculus | 26 | 67 |
| Q9HBH9 | hMKNK2 | CAMK | Homo sapiens | 166 | 490 |
| P49137 | hMK2 | CAMK | Homo sapiens | 249 | 1153 |
| P07332 | hFES | TK | Homo sapiens | 50 | 343 |
| Q9P1W9 | hPIM2 | CAMK | Homo sapiens | 195 | 637 |
| P27448 | hMARK3 | CAMK | Homo sapiens | 134 | 654 |
| P21127 | hPITSLREa | CMGC | Homo sapiens | 3 | 37 |
| Q86UE8 | hTLK2 | Other | Homo sapiens | 5 | 37 |
| Q9NYY3 | hPLK2 | Other | Homo sapiens | 27 | 39 |
| Q99558 | hMAP3K14 | STE | Homo sapiens | 1 | 9 |
| P07948 | hLYN | TK | Homo sapiens | 351 | 575 |
| Q13177 | hPAK2 | STE | Homo sapiens | 2 | 45 |
| Q13153 | hPAK1 | STE | Homo sapiens | 20 | 727 |
| O43353 | hRIPK2 | TKL | Homo sapiens | 9 | 32 |
| P09769 | hFGR | TK | Homo sapiens | 20 | 37 |
| P52564 | hMKK6 | STE | Homo sapiens | 3 | 50 |
| P45984 | hJNK2 | CMGC | Homo sapiens | 157 | 767 |
| Q9NQU5 | hPAK6 | STE | Homo sapiens | 3 | 39 |
| O14965 | hAURa | Other | Homo sapiens | 978 | 1113 |
| P07947 | hYES1 | TK | Homo sapiens | 49 | 45 |
| Q9Y2H9 | hMAST1 | AGC | Homo sapiens | 2 | 4 |
| P46734 | hMKK3 | STE | Homo sapiens | 2 | 44 |
| Q9H0K1 | hSNF1LK2 | CAMK | Homo sapiens | 25 | 36 |
| P51957 | hNEK4 | Other | Homo sapiens | 68 | 529 |
| P35590 | hTIE1 | TK | Homo sapiens | 13 | 28 |
| Q5VT25 | hCDC42BPA | AGC | Homo sapiens | 85 | 701 |
| Q9Y243 | hAKT3 | AGC | Homo sapiens | 133 | 869 |
| Q9Y6R4 | hMAP3K4 | STE | Homo sapiens | 3 | 39 |
| O00311 | hCDC7 | Other | Homo sapiens | 411 | 425 |
| Q04759 | hPKCt | AGC | Homo sapiens | 473 | 653 |
| Q8TDR2 | hSTK35 | Other | Homo sapiens | 1 | 5 |
| Q60737 | mCSNK2A1 | CMGC | Mus musculus | 4 | 6 |
| P06213 | hINSR | TK | Homo sapiens | 197 | 1107 |
| O94806 | hPKD3 | CAMK | Homo sapiens | 282 | 985 |
| Q99683 | hMAP3K5 | STE | Homo sapiens | 6 | 53 |
| Q60751 | rIGF1R | TK | Rattus norvegicus | 28 | 2 |
| Q9BUB5 | hMKNK1 | CAMK | Homo sapiens | 26 | 55 |
| Q6ZN16 | hMAP3K15 | STE | Homo sapiens | 14 | 21 |
| P16277 | mBLK | TK | Mus musculus | 5 | 5 |
| P90584 | plPfmrk | CMGC | Plasmodium falciparum | 15 | 111 |
| P29597 | hTYK2 | TK | Homo sapiens | 67 | 567 |
| P41241 | mCSK | TK | Mus musculus | 57 | 28 |
| P17612 | hPKAa | AGC | Homo sapiens | 351 | 1344 |
| P09217 | rPKCz | AGC | Rattus norvegicus | 66 | 27 |
| P11275 | rCAMK2A | CAMK | Rattus norvegicus | 3 | 9 |
| Q07912 | hTNK2 | TK | Homo sapiens | 124 | 282 |
| Q9HCP0 | hCSNK1G1 | CK1 | Homo sapiens | 92 | 538 |
| Q7L7X3 | hTAOK1 | STE | Homo sapiens | 127 | 764 |
| Q02156 | hPKCe | AGC | Homo sapiens | 214 | 521 |
| Q13164 | hERK5 | CMGC | Homo sapiens | 18 | 43 |
| Q9Y6M4 | hCSNK1G3 | CK1 | Homo sapiens | 64 | 498 |
| O95382 | hMAP3K6 | STE | Homo sapiens | 1 | 5 |
| P53355 | hDAPK1 | CAMK | Homo sapiens | 7 | 41 |
| P21803 | mFGFR2 | TK | Mus musculus | 11 | 18 |
| P37023 | hALK1 | TKL | Homo sapiens | 2 | 39 |
| P49761 | hCLK3 | CMGC | Homo sapiens | 7 | 70 |
| Q8N752 | hCSNK1A1L | CK1 | Homo sapiens | 3 | 35 |
| P16056 | mMET | TK | Mus musculus | 1 | 1 |
| P54646 | hPRKAA2 | CAMK | Homo sapiens | 7 | 82 |
| O00418 | hEEF2K | Other | Homo sapiens | 6 | 394 |
| Q9H093 | hNUAK2 | CAMK | Homo sapiens | 11 | 30 |
| Q15208 | hSTK38 | AGC | Homo sapiens | 1 | 6 |
| P17948 | hVEGFR1 | TK | Homo sapiens | 642 | 614 |
| P49841 | hGSK3b | CMGC | Homo sapiens | 1291 | 1479 |
| Q05397 | hFAK1 | TK | Homo sapiens | 195 | 778 |
| Q9UBE8 | hNLK | CMGC | Homo sapiens | 28 | 41 |
| Q14012 | hCAMK1 | CAMK | Homo sapiens | 21 | 709 |
| O95819 | hMAP4K4 | STE | Homo sapiens | 357 | 651 |
| P29322 | hEPHA8 | TK | Homo sapiens | 10 | 31 |
| Q56UN5 | hYSK4 | STE | Homo sapiens | 126 | 76 |
| Q64617 | rPKCh | AGC | Rattus norvegicus | 66 | 56 |
| P45985 | hMKK4 | STE | Homo sapiens | 6 | 43 |
| P51812 | hRSK2 | CAMK | Homo sapiens | 194 | 813 |
| P53667 | hLIMK1 | TKL | Homo sapiens | 122 | 647 |
| O15197 | hEPHB6 | TK | Homo sapiens | 3 | 4 |
| P06494 | rERBB2 | TK | Rattus norvegicus | 11 | 2 |
| P28482 | hERK2 | CMGC | Homo sapiens | 81 | 646 |
| O15146 | hMUSK | TK | Homo sapiens | 10 | 33 |
| Q16584 | hMAP3K11 | TKL | Homo sapiens | 38 | 44 |
| P51813 | hBMX | TK | Homo sapiens | 11 | 43 |
| O43781 | hDYRK3 | CMGC | Homo sapiens | 109 | 416 |
| O15075 | hDCAMKL1 | CAMK | Homo sapiens | 16 | 623 |
| O95835 | hLATS1 | AGC | Homo sapiens | 5 | 36 |
| Q9Y2U5 | hMAP3K2 | STE | Homo sapiens | 4 | 3 |
| Q8N568 | hDCAMKL2 | CAMK | Homo sapiens | 3 | 38 |
| O75582 | hMSK1 | AGC | Homo sapiens | 99 | 350 |
| Q96PF2 | hTSSK2 | CAMK | Homo sapiens | 29 | 480 |
| P08581 | hMET | TK | Homo sapiens | 128 | 788 |
| Q02111 | mPKCt | AGC | Mus musculus | 3 | 1 |
| P29376 | hLTK | TK | Homo sapiens | 111 | 251 |
| P17252 | hPKCa | AGC | Homo sapiens | 323 | 684 |
| P15208 | mINSR | TK | Mus musculus | 2 | 50 |
| Q13464 | hROCK1 | AGC | Homo sapiens | 562 | 854 |
| Q9NY57 | hSTK32B | AGC | Homo sapiens | 2 | 39 |
| Q14289 | hFAK2 | TK | Homo sapiens | 102 | 406 |
| P49185 | rJNK1 | CMGC | Rattus norvegicus | 7 | 4 |
| Q13188 | hSTK3 | STE | Homo sapiens | 208 | 628 |
| Q08345 | hDDR1 | TK | Homo sapiens | 20 | 24 |
| Q96KB5 | hPBK | Other | Homo sapiens | 27 | 557 |
| P25098 | hADRBK1 | AGC | Homo sapiens | 4 | 7 |
| P09216 | rPKCe | AGC | Rattus norvegicus | 72 | 58 |
| P10721 | hKIT | TK | Homo sapiens | 496 | 674 |
| Q00535 | hCDK5 | CMGC | Homo sapiens | 491 | 1263 |
| P29323 | hEPHB2 | TK | Homo sapiens | 11 | 78 |
| Q86UX6 | hSTK32C | AGC | Homo sapiens | 1 | 40 |
| P51955 | hNEK2 | Other | Homo sapiens | 113 | 863 |
| Q15746 | hMYLK | CAMK | Homo sapiens | 29 | 58 |
| P45983 | hJNK1 | CMGC | Homo sapiens | 501 | 1209 |
| O14976 | hGAK | Other | Homo sapiens | 23 | 23 |
| Q02763 | hTIE2 | TK | Homo sapiens | 416 | 323 |
| Q86YV6 | hSgK085 | CAMK | Homo sapiens | 6 | 35 |
| Q9NWZ3 | hIRAK4 | TKL | Homo sapiens | 163 | 725 |
| Q15375 | hEPHA7 | TK | Homo sapiens | 6 | 37 |
| Q13873 | hBMPR2 | TKL | Homo sapiens | 3 | 39 |
| P22607 | hFGFR3 | TK | Homo sapiens | 144 | 636 |
| Q9BQI3 | hHRI | Other | Homo sapiens | 20 | 8 |
| P05696 | rPKCa | AGC | Rattus norvegicus | 89 | 58 |
| Q16512 | hPKN1 | AGC | Homo sapiens | 8 | 36 |
| P05622 | mPDGFRb | TK | Mus musculus | 140 | 385 |
| P42685 | hFRK | TK | Homo sapiens | 170 | 358 |
| Q09013 | hDMPK | AGC | Homo sapiens | 5 | 44 |
| P18266 | rGSK3b | CMGC | Rattus norvegicus | 5 | 2 |
| Q8IU85 | hCAMK1D | CAMK | Homo sapiens | 43 | 321 |
| Q9UM73 | hALK | TK | Homo sapiens | 214 | 704 |
| P54764 | hEPHA4 | TK | Homo sapiens | 6 | 40 |
| Q14680 | hMELK | CAMK | Homo sapiens | 163 | 427 |
| Q9NRP7 | hSTK36 | Other | Homo sapiens | 4 | 38 |
| P16092 | mFGFR1 | TK | Mus musculus | 15 | 30 |
| P35918 | mVEGFR2 | TK | Mus musculus | 135 | 108 |
| Q4JIM5 | mABL2 | TK | Mus musculus | 2 | 2 |
| P36897 | hTGFbR1 | TKL | Homo sapiens | 262 | 181 |
| Q05513 | hPKCz | AGC | Homo sapiens | 121 | 1123 |
| P31750 | mAKT1 | AGC | Mus musculus | 1 | 5 |
| P54756 | hEPHA5 | TK | Homo sapiens | 8 | 36 |
| Q03142 | mFGFR4 | TK | Mus musculus | 11 | 18 |
| P43403 | hZAP70 | TK | Homo sapiens | 80 | 149 |
| Q16288 | hNTRK3 | TK | Homo sapiens | 197 | 511 |
| P00521 | mlvABL1 | TK | Mus musculus | 2 | 51 |

## 2.2 External testing dataset

Four different external datasets with diverse experimental methods and value types were used to evaluate the model. (1) Davis dataset. Published by Davis et al.(Davis, et al., 2011), Davis dataset contains 72 known inhibitors against a panel of 442 kinase assays, resulting in a total of 9,424 Kd values for all potential protein-ligand pairs. (2) Anastassiadis dataset. Anastassiadis et al.(Theonie, et al., 2011) reported the inhibitory percentage inhibition values of 178 compounds tested against 300 kinases at 0.5 μM. (3) Published Kinase Inhibitor Set 1(PKIS1)(Elkins, et al., 2015). PKIS1 is a collection of 367 kinase inhibitors representing 31 diverse chemotypes, and their inhibitory percentage values evaluated against 232 kinases at 1 μM were collected. (4) Published Kinase Inhibitor Set 2 (PKIS2)(Drewry, et al., 2017). PKIS2 is composed of 645 small-molecule inhibitors representing 86 diverse chemotypes, which were all profiled at a concentration of 1 μM against a broader panel of 392 kinases. For the dataset of Anastassiadis et al., the activity threshold is set by converting the single point activity with the equation previously defined(Sutherland, et al., 2013). For datasets PKIS1 and PKIS2, an inhibition rate over 50% at 1 µM was defined as signifying activity(Posy, et al., 2011). Note that all compound-kinase pairs included in our training dataset were removed from these external datasets before further evaluations.

# 3 Model performance

Extensive computational and experimental validations have been performed. The model shows excellent prediction ability with an auROC of 0.90 on an internal test dataset and impressive performance on four external datasets. To verify the generalizability and transfer learning effect of our MTDNN model, a parallel comparison with previously reported models was carried out. Here, we chose the random forest models (RFs) build by Merget et al. (Merget, et al., 2016) (<https://github.com/Team-SKI/Publications>). As shown in supplementary figure 2, the MTDNN showed consistently higher average auROC values than those of the RFs on all four external datasets and achieved more high-quality predictions than RFs. Moreover, the decent predictive capability of MTDNN for the kinases with insufficient activity data can be shown in supplementary table 2. The details of the validation can be found in <https://kinome.dddc.ac.cn/en/page/about/>.

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### Supplementary figure 2. Prediction performance comparison between MTDNN and RF of Merget et al. Barplots of auROCs for kinases, grouped by underlying external datasets and coloured by method (RF in red and MTDNN in blue).

### Supplementary table 2. Prediction performance comparison between MTDNN and RFs of Merget et al.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Kinase | Size of training dataset | | auROC | | | | | | | |
| Davis dataset | | Anastassiadis dataset | | PKIS1 | | PKIS2 | |
| Active sample | Inactive sample | RF | MTDNN | RF | MTDNN | RF | MTDNN | RF | MTDNN |
| Q9HAZ1 | 446 | 399 | 0.6206 | 0.6736 | 0.5952 | 0.7245 |  |  | 0.6543 | 0.6665 |
| P49760 | 203 | 537 | 0.6250 | 0.7071 | 0.5438 | 0.6599 | 0.5179 | 0.7767 | 0.5159 | 0.6671 |
| P36894 | 3 | 13 | 0.5417 | 0.8071 |  |  |  |  | 0.5000 | 0.7362 |
| Q59H18 | 1 | 15 | 0.5000 | 0.8083 |  |  |  |  | 0.5000 | 0.6170 |
| P80192 | 29 | 23 | 0.6000 | 0.6250 | 0.5641 | 0.6738 |  |  | 0.5000 | 0.7421 |
| Q9UQ88 | 2 | 14 | 0.5000 | 0.8368 |  |  |  |  | 0.5000 | 0.3783 |
| Q9Y4K4 | 192 | 337 | 0.6471 | 0.7435 | 0.6134 | 0.6773 |  |  | 0.6128 | 0.7368 |
| O00506 | 3 | 13 | 0.6159 | 0.5897 | 0.5769 | 0.7482 |  |  | 0.5000 | 0.7499 |
| Q14164 | 41 | 262 | 0.6111 | 0.8214 | 0.5556 | 0.6742 | 0.5000 | 0.5812 | 0.5000 | 0.6907 |
| P27361 | 78 | 273 | 0.5000 | 0.6341 | 0.5000 | 0.7041 | 0.4958 | 0.9719 | 0.5000 | 0.4996 |
| Q96RR4 | 10 | 31 | 0.5800 | 0.6364 | 0.6429 | 0.7477 |  |  | 0.5139 | 0.7120 |
| Q9H1R3 | 5 | 12 | 0.6011 | 0.8559 | 0.5917 | 0.8199 |  |  | 0.5000 | 0.7907 |
| P26618 | 22 | 76 |  |  |  |  |  |  |  |  |
| P15056 | 267 | 124 | 0.6044 | 0.7756 | 0.4469 | 0.6742 | 0.6528 | 0.7551 | 0.6364 | 0.6762 |
| Q9UKE5 | 3 | 13 | 0.5122 | 0.6119 |  |  |  |  | 0.5000 | 0.6902 |
| Q13470 | 3 | 13 | 0.5553 | 0.7642 |  |  | 0.5000 | 0.7023 | 0.5000 | 0.5254 |
| Q13627 | 264 | 617 | 0.6538 | 0.8576 | 0.6364 | 0.7070 | 0.5383 | 0.8073 | 0.5146 | 0.6890 |
| P42679 | 22 | 331 | 0.4914 | 0.9245 |  | 0.5227 |  |  | 0.5000 | 0.5945 |
| P11799 | 26 | 63 |  |  |  |  |  |  |  |  |
| P57059 | 4 | 13 | 0.5769 | 0.7930 |  |  | 0.5000 | 0.6619 | 0.5000 | 0.6832 |
| O14733 | 1 | 2 | 0.5000 | 0.3761 |  |  |  |  | 0.5000 | 0.2979 |
| Q96L34 | 11 | 24 | 0.7000 | 0.9797 | 0.6250 | 0.7170 | 0.4986 | 0.8486 | 0.5435 | 0.6617 |
| Q9H3Y6 | 32 | 340 | 0.5514 | 0.7095 | 0.4936 | 0.7319 | 0.5000 | 0.3412 | 0.5000 | 0.6775 |
| Q9Y616 | 2 | 14 | 0.5417 | 0.7353 |  |  |  |  | 0.5000 | 0.6122 |
| Q9BYT3 | 4 | 18 | 0.5667 | 0.7118 | 0.6071 | 0.7662 |  |  | 0.5000 | 0.7153 |
| P50613 | 105 | 285 | 0.6407 | 0.7233 | 0.7435 | 0.8306 |  |  | 0.5208 | 0.7210 |
| O15530 | 166 | 541 | 0.7398 | 0.7059 |  |  |  |  | 0.5673 | 0.7296 |
| O95747 | 1 | 2 | 0.4851 | 0.9846 | 0.4942 | 0.7415 |  |  | 0.5000 | 0.6749 |
| Q13882 | 33 | 294 | 0.5000 | 0.7419 | 0.5000 | 0.6125 | 0.5000 | 0.6835 | 0.5000 | 0.7877 |
| Q13554 | 48 | 498 | 0.7500 | 0.8586 | 0.6429 | 0.7523 |  |  | 0.5000 | 0.4563 |
| Q9WUI1 | 25 | 1 |  |  |  |  |  |  |  |  |
| P22694 | 46 | 365 | 0.5000 | 0.8816 |  |  |  |  | 0.5094 | 0.7154 |
| P00516 | 9 | 11 |  |  |  |  |  |  |  |  |
| O94804 | 5 | 12 | 0.5517 | 0.7895 | 0.5690 | 0.7169 | 0.5000 | 0.6845 | 0.5000 | 0.5340 |
| O14757 | 906 | 973 | 0.5894 | 0.6452 | 0.5385 | 0.7904 | 0.5000 | 0.6607 | 0.5000 | 0.6244 |
| O75385 | 2 | 2 | 0.6310 | 0.8393 | 0.5640 | 0.7552 |  |  | 0.5740 | 0.7200 |
| P04409 | 2 | 1 |  |  |  |  |  |  |  |  |
| P52333 | 125 | 578 | 0.6471 | 0.7772 | 0.5833 | 0.7814 | 0.4929 | 0.7914 |  |  |
| P70618 | 32 | 5 |  |  |  |  |  |  |  |  |
| P05771 | 210 | 364 |  |  | 0.9167 | 0.9024 |  |  |  |  |
| O75914 | 2 | 28 | 0.6111 | 0.7104 | 0.7000 | 0.8980 |  |  | 0.5000 | 0.6914 |
| P35916 | 210 | 472 | 0.6773 | 0.8932 | 0.5556 | 0.7892 | 0.5836 | 0.7601 | 0.6219 | 0.8101 |
| P49840 | 410 | 769 | 0.5556 | 0.6500 | 0.6823 | 0.9232 | 0.6320 | 0.9138 | 0.5721 | 0.7294 |
| Q92918 | 4 | 12 | 0.5372 | 0.6716 |  |  |  |  | 0.5000 | 0.7353 |
| P48730 | 129 | 472 | 0.6250 | 0.6042 | 0.6394 | 0.7696 |  |  | 0.5987 | 0.7894 |
| Q9H2X6 | 165 | 363 | 0.5214 | 0.6224 | 0.7436 | 0.7933 |  |  | 0.5164 | 0.6730 |
| Q8NFD2 | 3 | 13 | 0.5456 | 0.7793 |  |  |  |  | 0.5000 | 0.6476 |
| P42681 | 13 | 13 | 0.6276 | 0.8081 | 0.5987 | 0.7266 | 0.6124 | 0.6163 | 0.5316 | 0.6276 |
| P08631 | 156 | 125 | 0.5963 | 0.7367 | 0.6495 | 0.7202 | 0.5579 | 0.6664 | 0.4977 | 0.6602 |
| P53350 | 232 | 736 | 0.6000 | 1.0000 | 0.5000 | 0.5086 | 0.7813 | 0.9167 | 0.5968 | 0.7455 |
| P53779 | 272 | 307 | 0.6674 | 0.5628 |  | 0.4702 |  |  | 0.6133 | 0.6848 |
| Q64725 | 1 | 1 |  |  |  |  |  |  |  |  |
| Q6DT37 | 1 | 15 | 0.6000 | 0.7564 |  |  |  |  | 0.5000 | 0.4668 |
| P36896 | 3 | 13 | 0.5739 | 0.8423 | 0.4938 | 0.8294 |  |  | 0.5000 | 0.5639 |
| Q9BXA7 | 47 | 362 | 0.7402 | 0.9559 | 0.6154 | 0.6602 | 0.5206 | 0.8813 | 0.5000 | 0.6554 |
| Q9JI10 | 2 | 0 |  |  |  |  |  |  |  |  |
| Q92772 | 2 | 2 | 0.5330 | 0.5653 |  |  |  |  | 0.4946 | 0.6490 |
| Q06187 | 87 | 533 | 0.5989 | 0.8854 | 0.5789 | 0.7435 | 0.4959 | 0.2027 | 0.4983 | 0.6842 |
| Q9NR20 | 24 | 391 |  |  |  | 0.6687 |  |  |  |  |
| Q9Y6E0 | 3 | 13 | 0.5739 | 0.6250 | 0.6250 | 0.7440 |  |  | 0.5000 | 0.6616 |
| P16234 | 236 | 376 | 0.7000 | 0.8471 | 0.7429 | 0.7192 | 0.5887 | 0.7206 | 0.5694 | 0.7528 |
| Q96SB4 | 33 | 445 | 0.6139 | 0.5611 | 0.7467 | 0.5333 |  |  | 0.5000 | 0.5763 |
| P05480 | 13 | 8 |  |  |  |  |  |  |  |  |
| Q8TDX7 | 1 | 16 | 0.5000 | 0.6500 |  | 0.8000 |  |  | 0.5000 | 0.6584 |
| O75676 | 11 | 10 |  |  | 0.4938 | 0.7831 | 0.4830 | 0.9103 |  |  |
| Q8TD08 | 5 | 11 | 0.5310 | 0.6993 |  |  |  |  | 0.5000 | 0.7480 |
| Q13043 | 4 | 21 | 0.5727 | 0.6667 | 0.5556 | 0.7938 | 0.5000 | 0.8292 | 0.5083 | 0.6642 |
| Q15831 | 3 | 13 | 0.6667 | 0.7947 | 0.5633 | 0.6672 |  |  | 0.5000 | 0.6831 |
| Q13131 | 130 | 583 | 0.6364 | 0.7909 |  |  | 0.5000 | 0.8634 | 0.5135 | 0.7221 |
| P19525 | 3 | 14 | 0.6159 | 0.7833 |  |  |  |  | 0.5000 | 0.7201 |
| O14920 | 328 | 443 | 0.4904 | 0.5174 | 0.7467 | 0.8117 |  |  | 0.5128 | 0.7144 |
| Q96PY6 | 1 | 17 | 0.7500 | 0.8902 | 0.5556 | 0.6465 | 0.5000 | 0.4382 | 0.5000 | 0.5582 |
| Q8MMZ8 | 206 | 3 |  |  |  |  |  |  |  |  |
| P51817 | 161 | 459 | 0.8333 | 1.0000 | 0.6667 | 0.8303 | 0.5928 | 0.8728 | 0.5309 | 0.7837 |
| Q9UHD2 | 35 | 237 | 0.5714 | 0.6333 | 0.5667 | 0.7001 | 0.5000 | 0.7008 | 0.5125 | 0.6195 |
| Q13237 | 67 | 354 | 0.5714 | 0.8500 | 0.5455 | 0.6601 | 0.5208 | 0.8906 | 0.4983 | 0.7800 |
| P22455 | 21 | 58 | 0.6667 | 0.9352 | 0.6667 | 0.6054 |  |  | 0.5000 | 0.5846 |
| Q02750 | 325 | 352 | 0.6788 | 0.8333 | 0.8616 | 0.6387 | 0.4943 | 0.8870 | 0.5277 | 0.6657 |
| Q8N5S9 | 4 | 13 | 0.6250 | 0.7255 | 0.7500 | 0.7544 |  |  | 0.5000 | 0.7497 |
| Q9UPE1 | 2 | 3 | 0.6582 | 0.8728 | 0.5985 | 0.6543 | 0.5000 | 0.5275 | 0.5000 | 0.7441 |
| P05131 | 9 | 65 |  |  |  |  |  |  |  |  |
| P36888 | 513 | 617 | 0.7368 | 0.8792 | 0.6098 | 0.7116 | 0.6054 | 0.7167 | 0.6359 | 0.7619 |
| P20786 | 17 | 18 |  |  |  |  |  |  |  |  |
| Q9H4B4 | 60 | 491 | 0.5000 | 0.8986 | 0.5000 | 0.5181 |  |  | 0.5976 | 0.8375 |
| P04629 | 214 | 636 | 0.6000 | 0.8131 | 0.6139 | 0.7783 | 0.5677 | 0.9436 | 0.5099 | 0.6966 |
| O43283 | 2 | 2 | 0.4669 | 0.7060 |  |  |  |  | 0.4930 | 0.7073 |
| Q9UPZ9 | 2 | 2 | 0.6102 | 0.6374 |  |  |  |  | 0.4951 | 0.6898 |
| Q8IVH8 | 5 | 12 | 0.5821 | 0.7051 |  |  |  |  | 0.4974 | 0.7339 |
| P30530 | 127 | 233 | 0.7357 | 0.9161 | 0.6572 | 0.7993 | 0.8963 | 0.9107 | 0.5875 | 0.8093 |
| Q13555 | 70 | 460 | 0.7292 | 1.0000 | 0.6875 | 0.7868 |  |  | 0.5000 | 0.5202 |
| P33981 | 3 | 16 | 0.5714 | 0.7102 | 0.6968 | 0.7815 | 0.5000 | 0.7896 | 0.5000 | 0.6982 |
| Q86Z02 | 1 | 6 | 0.5000 | 0.6270 |  | 0.8514 | 0.5000 | 0.6269 | 0.5000 | 0.6521 |
| Q9BWU1 | 15 | 160 | 0.5714 | 0.7167 |  |  |  |  |  |  |
| O14578 | 2 | 15 | 0.5276 | 0.8929 |  |  |  |  | 0.5000 | 0.5367 |
| P11802 | 477 | 485 | 0.7576 | 0.8249 | 0.7283 | 0.7941 | 0.6029 | 0.7789 | 0.5463 | 0.6732 |
| P07949 | 250 | 462 | 0.6916 | 0.8654 | 0.6208 | 0.7334 | 0.6552 | 0.7868 | 0.6591 | 0.7781 |
| Q9WUD9 | 15 | 14 |  |  |  |  |  |  |  |  |
| Q9C098 | 2 | 14 | 0.5417 | 0.7898 |  |  |  |  | 0.5000 | 0.6844 |
| P21802 | 49 | 65 | 0.6439 | 0.9256 | 0.6634 | 0.8328 | 0.5000 | 0.6316 | 0.5000 | 0.6854 |
| P09215 | 54 | 44 |  |  |  |  |  |  |  |  |
| Q96NX5 | 2 | 13 | 0.5911 | 0.8400 | 0.7500 | 0.8444 |  |  | 0.5000 | 0.6138 |
| P63086 | 1 | 9 |  |  |  |  |  |  |  |  |
| Q5S007 | 99 | 178 | 0.6813 | 0.7762 | 0.6014 | 0.7350 | 0.7079 | 0.8645 | 0.5160 | 0.6262 |
| O60674 | 136 | 518 | 0.6667 | 0.8333 | 0.5734 | 0.8194 | 0.6250 | 0.8125 |  |  |
| Q00537 | 3 | 13 | 0.5350 | 0.6503 |  |  |  |  | 0.5000 | 0.7092 |
| Q8IW41 | 27 | 393 | 0.5000 | 0.8286 | 0.5000 | 0.4996 |  |  | 0.5000 | 0.5040 |
| Q16620 | 128 | 601 | 0.6333 | 0.7971 | 0.6318 | 0.7167 | 0.5800 | 0.8730 | 0.5146 | 0.7194 |
| P49759 | 27 | 26 | 0.5682 | 0.6902 | 0.6981 | 0.6917 |  |  | 0.5000 | 0.7499 |
| P06493 | 670 | 1302 |  |  | 0.7267 | 0.7364 | 0.6041 | 0.8673 |  |  |
| P16591 | 91 | 281 | 0.6651 | 0.8795 | 0.6359 | 0.7063 | 0.7062 | 0.9472 | 0.5152 | 0.7317 |
| P23443 | 220 | 412 | 0.5944 | 0.7840 | 0.6047 | 0.7414 | 0.9240 | 0.9297 | 0.5410 | 0.8186 |
| Q9H422 | 3 | 1 | 0.5000 | 0.6894 | 0.5000 | 0.6290 |  |  | 0.5000 | 0.6688 |
| P49674 | 11 | 25 | 0.5509 | 0.6034 | 0.5611 | 0.7372 |  |  | 0.5000 | 0.5973 |
| P27037 | 1 | 15 | 0.5000 | 0.7083 |  |  |  |  | 0.5000 | 0.5838 |
| Q9UIK4 | 2 | 17 | 0.5556 | 0.7500 | 0.6218 | 0.6414 |  |  | 0.5000 | 0.6256 |
| Q16513 | 145 | 421 | 0.7500 | 0.7917 | 0.6966 | 0.7804 |  |  | 0.5392 | 0.8347 |
| Q02779 | 19 | 30 | 0.8333 | 0.5641 | 0.6667 | 0.8239 |  |  | 0.5357 | 0.6843 |
| P78368 | 68 | 417 | 0.5000 | 0.8384 | 0.5966 | 0.6150 | 0.5000 | 0.7375 | 0.5185 | 0.6664 |
| Q13546 | 3 | 15 | 0.4902 | 0.2474 |  |  |  |  | 0.5000 | 0.4294 |
| O43293 | 202 | 556 | 0.7273 | 0.8889 | 0.7965 | 0.7420 |  |  | 0.5290 | 0.6677 |
| XP\_341554.1 | 54 | 44 |  |  |  |  |  |  |  |  |
| Q9UQM7 | 49 | 322 | 0.6667 | 0.8276 | 0.6250 | 0.7177 | 0.5000 | 0.7918 | 0.5000 | 0.4763 |
| P41743 | 79 | 591 | 0.4833 | 0.9630 | 0.7437 | 0.7919 | 1.0000 | 0.9973 | 0.5000 | 0.5964 |
| Q13705 | 1 | 16 | 0.5000 | 0.6333 |  |  |  |  | 0.5000 | 0.6517 |
| Q05655 | 76 | 486 | 0.5000 | 0.8639 | 0.5000 | 0.7500 |  |  | 0.5000 | 0.8374 |
| Q15139 | 74 | 233 | 0.4700 | 0.5551 | 0.6393 | 0.7308 | 0.5000 | 0.8180 | 0.5000 | 0.6606 |
| Q8IVW4 | 2 | 2 | 0.5606 | 0.8231 |  |  |  |  | 0.4906 | 0.5992 |
| Q15303 | 65 | 480 | 0.6250 | 0.9231 | 0.6041 | 0.7372 | 0.6350 | 0.9069 | 0.5479 | 0.7526 |
| Q16566 | 4 | 32 | 0.5907 | 0.8474 | 0.9938 | 0.9941 |  |  | 0.5000 | 0.7625 |
| P06239 | 952 | 1177 | 0.7130 | 0.9167 | 0.6959 | 0.7706 | 0.5656 | 0.6890 | 0.5848 | 0.7289 |
| P54753 | 9 | 31 | 0.5000 | 0.7566 | 0.5000 | 0.5097 | 0.5000 | 0.4046 | 0.5000 | 0.6580 |
| P51451 | 160 | 319 | 0.6250 | 0.9094 | 0.6142 | 0.7263 | 0.5385 | 0.6584 | 0.5675 | 0.7199 |
| O15264 | 185 | 638 | 0.7304 | 0.8175 |  | 0.9299 |  |  | 0.5089 | 0.6116 |
| P63319 | 95 | 92 |  |  |  |  |  |  |  |  |
| Q00534 | 2 | 33 |  |  | 0.5247 | 0.7012 | 0.5000 | 0.8096 |  |  |
| O76039 | 1 | 3 | 0.5833 | 0.5972 |  |  |  |  | 0.5000 | 0.7491 |
| P08922 | 95 | 281 | 0.7898 | 0.8732 | 0.5591 | 0.7357 | 0.7285 | 0.7988 | 0.6520 | 0.6927 |
| O00141 | 87 | 547 |  |  | 0.6111 | 0.7494 | 0.4986 | 0.8080 | 0.4992 | 0.7407 |
| O94768 | 4 | 12 | 0.6572 | 0.9054 |  |  |  |  | 0.5000 | 0.7594 |
| P22612 | 44 | 348 |  |  | 0.6667 | 0.8864 |  |  |  |  |
| Q15569 | 3 | 13 | 0.5739 | 0.7568 |  |  |  |  | 0.5000 | 0.6470 |
| P21709 | 6 | 13 | 0.5310 | 0.7715 | 0.5737 | 0.5859 |  |  | 0.5000 | 0.6840 |
| Q9P289 | 3 | 20 | 0.5618 | 0.6171 | 0.5388 | 0.6606 | 0.5000 | 0.9541 | 0.5000 | 0.6748 |
| Q15835 | 2 | 2 | 0.4350 | 0.4298 |  |  |  |  | 0.5347 | 0.4008 |
| Q06418 | 80 | 526 | 0.5894 | 0.8067 | 0.7143 | 0.6455 | 0.5000 | 0.8593 | 0.5000 | 0.6084 |
| Q9UKI8 | 3 | 13 | 0.6907 | 0.6526 |  |  |  |  | 0.5000 | 0.6804 |
| Q7KZI7 | 80 | 418 | 0.6769 | 0.8940 | 0.6214 | 0.7636 | 0.5000 | 0.8284 | 0.4992 | 0.7266 |
| Q16644 | 7 | 556 |  |  |  | 0.4055 |  |  |  |  |
| P00533 | 1405 | 1793 | 0.7375 | 0.8400 | 0.8750 | 0.8267 | 0.8935 | 0.9350 | 0.6054 | 0.6941 |
| O75116 | 551 | 481 | 0.5767 | 0.7262 | 0.6562 | 0.7656 | 0.6038 | 0.9005 | 0.6998 | 0.7787 |
| P34947 | 34 | 257 |  |  | 1.0000 | 0.7649 |  |  |  |  |
| P07333 | 479 | 636 | 0.7092 | 0.8138 | 0.6006 | 0.7226 | 0.5702 | 0.6904 | 0.5611 | 0.7545 |
| Q00536 | 3 | 13 | 0.5769 | 0.8061 |  |  |  |  | 0.5000 | 0.7172 |
| P11362 | 379 | 1018 | 0.6361 | 0.9203 | 0.5872 | 0.7100 | 0.4972 | 0.9652 | 0.5369 | 0.6677 |
| Q9Y5S2 | 2 | 15 | 0.5907 | 0.5641 | 0.7469 | 0.7928 | 0.5000 | 0.6732 | 0.5000 | 0.5737 |
| Q99640 | 1 | 16 | 0.5000 | 0.9756 |  |  |  |  | 0.5000 | 0.4650 |
| P00517 | 20 | 72 |  |  |  |  |  |  |  |  |
| Q9HC98 | 1 | 26 | 0.5000 | 0.5705 |  | 0.6842 |  |  | 0.5000 | 0.6817 |
| Q9Y463 | 106 | 225 | 0.7000 | 0.7222 | 0.6036 | 0.6950 | 0.4970 | 0.8420 | 0.5037 | 0.6307 |
| P54762 | 4 | 12 | 0.5350 | 0.7680 | 0.5523 | 0.7211 |  |  | 0.5000 | 0.6539 |
| Q16816 | 31 | 30 | 0.6000 | 0.6929 | 0.5909 | 0.7160 | 0.5000 | 0.7890 | 0.5000 | 0.7460 |
| P09619 | 386 | 673 | 0.6764 | 0.9555 | 0.6523 | 0.6721 | 0.5787 | 0.6470 | 0.5369 | 0.7252 |
| P08069 | 467 | 882 | 0.6250 | 0.5300 | 0.5833 | 0.5438 | 0.7308 | 0.9339 | 0.5609 | 0.7828 |
| P15735 | 72 | 428 | 0.6320 | 0.7734 | 0.7143 | 0.8184 | 0.5000 | 0.8273 | 0.5000 | 0.7946 |
| Q9UEW8 | 2 | 2 | 0.6425 | 0.8222 | 0.6156 | 0.5776 |  |  | 0.5168 | 0.7394 |
| P06241 | 168 | 305 | 0.5654 | 0.8240 | 0.5715 | 0.7699 | 0.5626 | 0.6896 | 0.5352 | 0.7295 |
| Q9NYL2 | 37 | 452 | 0.5000 | 0.5491 | 0.5000 | 0.6688 |  |  | 0.5000 | 0.5573 |
| P24941 | 1348 | 1375 | 0.8306 | 1.0000 | 0.8091 | 0.8867 | 0.8151 | 0.8627 | 0.7676 | 0.6384 |
| P41240 | 11 | 36 | 0.5739 | 0.8757 | 0.6429 | 0.6865 | 0.5000 | 0.4962 | 0.5000 | 0.6710 |
| Q96Q40 | 1 | 3 | 0.5000 | 0.5151 |  |  |  |  | 0.5000 | 0.3539 |
| O75716 | 3 | 13 | 0.6071 | 0.8038 | 0.5967 | 0.7202 |  |  | 0.5000 | 0.7078 |
| Q9P0L2 | 2 | 16 | 0.6667 | 0.9474 | 0.5833 | 0.8115 | 0.5000 | 0.7250 | 0.5000 | 0.6642 |
| Q04771 | 60 | 234 | 0.5603 | 0.8520 | 0.4936 | 0.4938 |  |  | 0.5000 | 0.7217 |
| Q04912 | 87 | 211 | 0.7398 | 0.9550 | 0.9873 | 0.5852 | 0.5000 | 0.6149 | 0.5239 | 0.6700 |
| Q8TDC3 | 44 | 435 | 0.6467 | 0.9192 | 0.5789 | 0.8559 | 0.4957 | 0.8151 | 0.5000 | 0.6102 |
| P00523 | 110 | 68 |  |  |  |  |  |  |  |  |
| P11309 | 307 | 856 | 0.7857 | 0.9333 | 0.6922 | 0.8354 | 0.5790 | 0.7754 | 0.4967 | 0.7298 |
| Q9Y2H1 | 3 | 13 | 0.7412 | 0.9878 |  |  |  |  | 0.5000 | 0.7727 |
| Q13976 | 94 | 332 | 0.7500 | 0.5000 | 0.7500 | 0.8051 | 0.5236 | 0.8864 | 0.5304 | 0.8348 |
| Q9NZJ5 | 12 | 11 |  |  |  |  |  |  |  |  |
| P32298 | 2 | 2 | 0.5774 | 0.8357 | 0.5643 | 0.8795 |  |  | 0.5570 | 0.7821 |
| P0C264 | 1 | 3 | 0.5753 | 0.8333 |  |  |  |  | 0.5000 | 0.6439 |
| Q6PHR2 | 2 | 2 | 0.4704 | 0.7359 | 0.5674 | 0.7633 |  |  | 0.3870 | 0.7113 |
| Q9H2K8 | 2 | 3 | 0.5646 | 0.7489 | 0.6636 | 0.8319 |  |  | 0.5000 | 0.7366 |
| Q9UQB9 | 19 | 20 | 0.6436 | 0.9677 | 0.5839 | 0.8333 | 0.5851 | 0.7847 | 0.5618 | 0.7472 |
| P14616 | 2 | 14 | 0.5625 | 0.6929 | 0.6111 | 0.7359 | 0.5000 | 0.6778 | 0.5000 | 0.6897 |
| P49187 | 29 | 36 |  |  |  |  |  |  |  |  |
| Q6P3R8 | 1 | 14 | 0.6250 | 0.9125 |  |  |  |  | 0.5000 | 0.5998 |
| P68400 | 123 | 599 | 0.4900 | 0.8485 | 0.5000 | 0.6529 | 0.4972 | 0.5350 | 0.5000 | 0.6283 |
| P04626 | 604 | 833 | 0.5000 | 0.7097 | 0.8182 | 0.8808 | 0.9460 | 0.9597 | 0.6164 | 0.6639 |
| O00444 | 158 | 401 | 0.6424 | 0.8636 |  |  |  |  | 0.6024 | 0.7577 |
| P47811 | 159 | 30 |  |  |  |  |  |  |  |  |
| P31749 | 616 | 880 | 0.8333 | 0.9697 | 1.0000 | 0.8882 | 0.9901 | 0.9423 | 0.8525 | 0.9341 |
| P36507 | 53 | 236 | 0.5256 | 0.7470 | 0.9967 | 0.6449 |  |  | 0.5000 | 0.6965 |
| Q01279 | 9 | 45 |  |  |  |  |  |  |  |  |
| P51617 | 65 | 391 | 0.5714 | 0.7131 | 0.5875 | 0.6791 |  |  | 0.5119 | 0.6703 |
| P50750 | 141 | 254 | 0.7391 | 0.9194 | 0.6181 | 0.7376 |  |  | 0.5351 | 0.6055 |
| Q8NEV4 | 2 | 14 | 0.5907 | 0.9231 |  |  |  |  | 0.5000 | 0.6060 |
| Q08881 | 350 | 509 | 0.5767 | 0.9107 | 0.6596 | 0.6426 | 0.4890 | 0.9613 | 0.5225 | 0.6875 |
| O15111 | 91 | 382 | 0.4898 | 0.8000 | 1.0000 | 0.8398 | 0.5000 | 0.6913 | 0.5000 | 0.6218 |
| Q92630 | 2 | 4 | 0.5591 | 0.8139 | 0.5363 | 0.7512 | 0.5000 | 0.7129 | 0.5000 | 0.7484 |
| Q9H2G2 | 131 | 352 | 0.5769 | 0.8618 | 0.5938 | 0.7894 |  |  | 0.5609 | 0.6996 |
| P00519 | 586 | 548 | 0.6488 | 0.8684 | 0.5853 | 0.8169 | 0.5886 | 0.7678 | 0.5772 | 0.6856 |
| P04049 | 207 | 113 | 0.7604 | 0.7500 | 0.8994 | 0.5712 | 0.8243 | 0.9057 | 0.6906 | 0.7033 |
| Q13557 | 63 | 425 | 0.5714 | 0.9544 | 0.5385 | 0.7715 | 0.5000 | 0.8503 | 0.4992 | 0.6082 |
| P30291 | 189 | 74 | 0.7500 | 0.7895 | 0.7375 | 0.6154 |  |  | 0.5824 | 0.5836 |
| Q8IYT8 | 2 | 2 | 0.5350 | 0.7547 | 0.6364 | 0.7954 |  |  | 0.5179 | 0.8047 |
| Q2M2I8 | 3 | 13 | 0.5938 | 0.8256 |  |  |  |  | 0.5000 | 0.7575 |
| P05129 | 190 | 830 |  |  | 0.9965 | 0.8171 | 0.6653 | 0.9751 |  |  |
| P42684 | 49 | 69 | 0.6111 | 0.8074 | 0.5641 | 0.7664 | 0.5000 | 0.7090 | 0.5082 | 0.7958 |
| P12931 | 1159 | 1440 | 0.7605 | 0.8182 | 0.7019 | 0.7911 | 0.5246 | 0.7045 | 0.5809 | 0.7634 |
| P29320 | 7 | 16 | 0.5350 | 0.7026 | 0.5936 | 0.8487 | 0.5700 | 0.6825 | 0.5000 | 0.6303 |
| Q9Y2K2 | 1 | 2 | 0.6667 | 0.7387 |  |  |  |  | 0.5000 | 0.5632 |
| O96017 | 209 | 472 | 0.5402 | 0.6593 | 0.5793 | 0.7355 | 0.5000 | 0.8559 | 0.5066 | 0.6440 |
| XP\_620754.3 | 2 | 1 |  |  |  |  |  |  |  |  |
| O96013 | 95 | 751 | 0.6560 | 0.9333 | 0.8333 | 0.6972 |  |  | 0.5000 | 0.8231 |
| P53671 | 31 | 21 | 0.4907 | 0.6538 |  |  |  |  | 0.5000 | 0.6831 |
| Q8NE63 | 118 | 352 | 0.5714 | 0.6853 | 0.4968 | 0.6498 | 0.6133 | 0.6621 | 0.5649 | 0.6827 |
| P68403 | 73 | 44 |  |  |  |  |  |  |  |  |
| P54760 | 154 | 207 | 0.4608 | 0.8971 | 0.5648 | 0.8696 | 0.6121 | 0.8367 | 0.5211 | 0.7784 |
| Q86V86 | 84 | 401 | 0.6667 | 0.6667 | 0.5714 | 0.7580 | 0.5000 | 0.7483 | 0.5362 | 0.8004 |
| P48729 | 104 | 663 | 0.5833 | 0.6768 | 0.4965 | 0.6421 | 0.6407 | 0.8797 | 0.5823 | 0.7353 |
| P53778 | 195 | 647 | 0.7194 | 0.7647 |  | 0.3878 | 0.4958 | 0.8028 | 0.5229 | 0.4974 |
| Q96GD4 | 587 | 675 | 0.8690 | 0.9954 | 0.7156 | 0.7679 | 0.7217 | 0.7836 | 0.6648 | 0.8060 |
| P05132 | 1 | 7 |  |  |  |  |  |  |  |  |
| P06240 | 32 | 43 |  |  |  |  |  |  |  |  |
| P00520 | 4 | 3 |  |  |  |  |  |  |  |  |
| Q8N4C8 | 136 | 366 | 0.6111 | 0.7857 | 0.6053 | 0.7380 | 0.5060 | 0.7889 | 0.5171 | 0.7030 |
| Q16539 | 1751 | 915 | 0.8741 | 0.9167 | 0.9746 | 0.8127 | 0.8529 | 0.9104 | 0.7097 | 0.7379 |
| P29317 | 80 | 478 | 0.5000 | 0.8424 | 0.5000 | 0.7834 | 0.6471 | 0.8415 | 0.5108 | 0.7817 |
| Q9BZL6 | 100 | 468 | 0.5787 | 0.4688 | 0.6154 | 0.6419 | 0.5000 | 0.8903 | 0.5161 | 0.6468 |
| Q9NSY1 | 3 | 13 | 0.5833 | 0.7238 |  |  |  |  | 0.5000 | 0.7908 |
| Q8WTQ7 | 2 | 2 | 0.6607 | 0.8314 | 0.5740 | 0.8400 | 0.6379 | 0.8587 | 0.6383 | 0.7776 |
| Q61851 | 8 | 13 |  |  |  |  |  |  |  |  |
| Q16659 | 1 | 15 | 0.5000 | 0.5238 |  |  |  |  | 0.5000 | 0.6097 |
| P19784 | 18 | 118 | 0.5000 | 0.6654 | 0.4963 | 0.6395 |  |  | 0.5000 | 0.6258 |
| Q8IY84 | 1 | 6 |  |  |  |  |  |  | 0.5000 | 0.6345 |
| Q8WXR4 | 2 | 14 | 0.6159 | 0.7417 | 0.6250 | 0.7544 |  |  | 0.5000 | 0.5485 |
| Q00526 | 3 | 43 | 0.5907 | 0.8583 | 0.5769 | 0.6657 | 0.5000 | 0.8969 | 0.5000 | 0.7309 |
| Q9UEE5 | 159 | 304 | 0.5583 | 0.5499 | 0.6169 | 0.7916 |  |  | 0.5243 | 0.6798 |
| Q9P286 | 3 | 13 | 0.5429 | 0.8612 | 0.6635 | 0.6167 | 0.5000 | 0.8493 | 0.5000 | 0.7748 |
| P70336 | 1 | 2 |  |  |  |  |  |  |  |  |
| P43405 | 225 | 454 | 0.6599 | 0.9375 | 0.6495 | 0.7367 | 0.7154 | 0.7590 | 0.5940 | 0.6852 |
| P35968 | 2097 | 1785 | 0.7835 | 0.7619 | 0.7063 | 0.7166 | 0.6619 | 0.7218 | 0.6378 | 0.7839 |
| P35969 | 12 | 50 |  |  |  |  |  |  |  |  |
| Q9UBS0 | 11 | 10 |  |  | 0.8721 | 0.8231 |  |  |  |  |
| P31751 | 263 | 652 | 1.0000 | 1.0000 | 0.7466 | 0.8952 | 0.9958 | 0.9977 | 0.7611 | 0.8083 |
| P49336 | 114 | 243 | 0.8116 | 0.9242 |  |  |  |  | 0.5557 | 0.5876 |
| O00238 | 1 | 2 | 0.5266 | 0.7062 |  |  |  |  | 0.5000 | 0.6615 |
| Q99759 | 2 | 3 | 0.5433 | 0.7242 | 0.7574 | 0.7306 |  |  | 0.5000 | 0.7435 |
| Q12851 | 196 | 512 | 0.5714 | 0.5406 | 0.5476 | 0.7407 | 0.5791 | 0.9550 | 0.5538 | 0.7491 |
| O60285 | 3 | 29 | 0.5455 | 0.8464 | 0.5250 | 0.7004 | 0.5227 | 0.8383 | 0.5000 | 0.7714 |
| Q96RG2 | 12 | 51 |  |  | 0.4969 | 0.7427 | 0.5000 | 0.9918 |  |  |
| P11440 | 21 | 54 |  |  |  |  |  |  |  |  |
| Q9HBH9 | 135 | 361 | 0.6500 | 0.9222 | 0.5519 | 0.7585 | 0.5763 | 0.5996 | 0.5101 | 0.6629 |
| P49137 | 196 | 858 | 0.9902 | 1.0000 | 1.0000 | 0.9968 |  |  | 0.5714 | 0.5421 |
| P07332 | 37 | 261 | 0.5385 | 0.9116 | 0.5556 | 0.6542 | 0.5000 | 0.8913 | 0.4992 | 0.7140 |
| Q9P1W9 | 152 | 470 | 0.6563 | 0.7688 | 0.5730 | 0.8561 | 0.5000 | 0.7582 | 0.5385 | 0.7537 |
| P27448 | 100 | 492 | 0.7000 | 0.7823 | 0.6630 | 0.8156 | 0.5000 | 0.8428 | 0.5345 | 0.7684 |
| P21127 | 1 | 15 | 0.5000 | 0.7263 |  |  |  |  | 0.5000 | 0.4262 |
| Q86UE8 | 3 | 14 | 0.8244 | 0.9583 | 0.6938 | 0.8509 |  |  | 0.5000 | 0.7791 |
| Q9NYY3 | 23 | 28 | 0.5754 | 0.6148 | 0.4885 | 0.5639 |  |  | 0.5000 | 0.6472 |
| Q99558 | 1 | 8 |  |  | 0.5000 | 0.6660 |  |  | 0.5000 | 0.5751 |
| P07948 | 272 | 434 | 0.6894 | 0.9762 | 0.6634 | 0.8539 |  |  | 0.6312 | 0.7521 |
| Q13177 | 2 | 19 | 0.6159 | 0.7436 | 0.7000 | 0.6297 |  |  | 0.5000 | 0.7449 |
| Q13153 | 17 | 548 | 0.6250 | 0.8889 | 0.5833 | 0.8960 |  |  | 0.5000 | 0.7512 |
| O43353 | 4 | 12 | 0.5333 | 0.7301 | 0.5227 | 0.6265 |  |  | 0.5000 | 0.5298 |
| P09769 | 11 | 19 | 0.5622 | 0.8606 | 0.5855 | 0.7612 | 0.5318 | 0.6844 | 0.5097 | 0.6907 |
| P52564 | 2 | 23 | 0.6577 | 0.8750 | 0.7500 | 0.7537 |  |  | 0.5000 | 0.6377 |
| P45984 | 116 | 600 | 0.6500 | 0.7959 | 0.4965 | 0.6041 | 0.4942 | 0.9437 | 0.5079 | 0.7135 |
| Q9NQU5 | 2 | 14 | 0.6159 | 0.9744 | 0.8333 | 0.5356 | 0.5000 | 0.8796 | 0.5000 | 0.7340 |
| O14965 | 766 | 868 | 0.7636 | 0.9821 | 0.6825 | 0.7454 | 0.6559 | 0.7710 | 0.6706 | 0.6820 |
| P07947 | 34 | 25 | 0.5502 | 0.7986 | 0.6403 | 0.7590 | 0.5162 | 0.6211 | 0.5390 | 0.7034 |
| Q9Y2H9 | 2 | 1 | 0.5000 | 0.8323 |  |  |  |  | 0.5008 | 0.4549 |
| P46734 | 2 | 17 | 0.5527 | 0.7893 |  |  |  |  | 0.5000 | 0.7807 |
| Q9H0K1 | 17 | 18 | 0.5556 | 0.7857 | 0.5187 | 0.7553 | 0.6303 | 0.5269 | 0.4847 | 0.6728 |
| P51957 | 49 | 408 | 0.5000 | 0.5000 | 0.5000 | 0.6689 |  |  | 0.5000 | 0.8355 |
| P35590 | 4 | 12 | 0.5156 | 0.7876 |  |  |  |  | 0.5000 | 0.6406 |
| Q5VT25 | 70 | 515 | 0.7402 | 0.5294 | 1.0000 | 0.6658 | 0.4986 | 0.9040 | 0.5000 | 0.6976 |
| Q9Y243 | 111 | 656 | 0.8333 | 0.8485 | 0.6250 | 0.7291 | 0.9271 | 0.8694 | 0.6875 | 0.8700 |
| Q9Y6R4 | 1 | 15 | 0.5000 | 0.6496 |  |  |  |  | 0.5000 | 0.5327 |
| O00311 | 319 | 322 |  |  |  |  |  |  |  |  |
| Q04759 | 374 | 509 | 0.8750 | 0.9417 | 0.8298 | 0.7157 | 0.4972 | 0.9754 | 0.5102 | 0.7607 |
| Q8TDR2 | 1 | 3 | 0.5216 | 0.5375 |  |  |  |  | 0.5000 | 0.6001 |
| Q60737 | 2 | 6 |  |  |  |  |  |  |  |  |
| P06213 | 151 | 849 | 0.6312 | 0.8571 | 0.6075 | 0.5953 | 0.7381 | 0.9296 | 0.5527 | 0.6818 |
| O94806 | 227 | 757 | 0.6509 | 0.6971 | 0.6176 | 0.7266 | 0.5206 | 0.8863 | 0.5371 | 0.6207 |
| Q99683 | 3 | 25 | 0.9915 | 1.0000 | 0.7000 | 0.8882 |  |  | 0.5000 | 0.7464 |
| Q60751 | 22 | 2 |  |  |  |  |  |  |  |  |
| Q9BUB5 | 20 | 28 | 0.7635 | 0.8829 | 0.8264 | 0.6253 | 0.4958 | 0.3496 | 0.5123 | 0.6783 |
| Q6ZN16 | 10 | 13 | 0.5841 | 0.7464 |  |  |  |  | 0.4967 | 0.4923 |
| P16277 | 3 | 4 |  |  |  |  |  |  |  |  |
| P90584 | 8 | 89 |  |  |  |  |  |  |  |  |
| P29597 | 45 | 435 | 0.5000 | 0.8075 | 0.5000 | 0.7421 | 0.5000 | 0.8722 |  |  |
| P41241 | 43 | 22 |  |  |  |  |  |  |  |  |
| P17612 | 279 | 1042 | 0.6000 | 0.8387 | 0.6250 | 0.8232 | 0.5833 | 0.8617 | 0.5326 | 0.7982 |
| P09217 | 54 | 18 |  |  |  |  |  |  |  |  |
| P11275 | 1 | 9 |  |  |  |  |  |  |  |  |
| Q07912 | 102 | 225 | 0.7000 | 0.9152 | 0.5323 | 0.6474 | 0.5000 | 0.7997 | 0.5296 | 0.6965 |
| Q9HCP0 | 77 | 393 | 0.5000 | 0.9714 | 0.4933 | 0.6242 | 0.4944 | 0.6156 | 0.5219 | 0.4889 |
| Q7L7X3 | 103 | 597 | 0.5506 | 0.6571 | 0.6250 | 0.7780 |  |  | 0.5152 | 0.6592 |
| Q02156 | 171 | 396 | 0.6875 | 0.8784 | 0.8501 | 0.8559 |  |  | 0.5000 | 0.8031 |
| Q13164 | 13 | 18 | 0.4906 | 0.7588 |  |  |  |  | 0.4968 | 0.5579 |
| Q9Y6M4 | 48 | 367 | 0.5000 | 0.9722 | 0.5801 | 0.6713 | 0.5000 | 0.5000 | 0.5172 | 0.4757 |
| O95382 | 1 | 3 | 0.9925 | 1.0000 |  |  |  |  | 0.5000 | 0.5212 |
| P53355 | 3 | 18 | 0.5398 | 0.7843 | 0.6875 | 0.5518 | 0.5000 | 0.9562 | 0.5000 | 0.6773 |
| P21803 | 8 | 13 |  |  |  |  |  |  |  |  |
| P37023 | 1 | 15 | 0.5000 | 0.7885 | 0.5000 | 0.4963 |  |  | 0.5000 | 0.6013 |
| P49761 | 3 | 37 | 0.5714 | 0.6984 | 0.4967 | 0.5519 | 0.5000 | 0.8315 | 0.5000 | 0.5941 |
| Q8N752 | 2 | 12 | 0.9917 | 1.0000 |  |  |  |  | 0.5000 | 0.7422 |
| P16056 | 1 | 0 |  |  |  |  |  |  |  |  |
| P54646 | 3 | 47 | 0.5909 | 0.7614 |  |  | 0.5000 | 0.8834 | 0.5000 | 0.7942 |
| O00418 | 3 | 306 |  |  |  |  |  |  |  |  |
| Q9H093 | 3 | 13 | 0.5750 | 0.7014 | 0.6396 | 0.6863 |  |  | 0.5000 | 0.7568 |
| Q15208 | 1 | 3 | 0.6000 | 0.8656 | 0.4946 | 0.6292 |  |  | 0.5000 | 0.5119 |
| P17948 | 506 | 505 | 0.6719 | 0.8550 | 0.6989 | 0.7081 | 0.6755 | 0.6793 | 0.6537 | 0.7786 |
| P49841 | 1018 | 1173 | 0.6417 | 0.6560 | 0.8249 | 0.8604 | 0.7863 | 0.9166 | 0.6714 | 0.6939 |
| Q05397 | 160 | 607 | 0.7857 | 0.8654 | 0.6250 | 0.6777 |  |  | 0.5644 | 0.6208 |
| Q9UBE8 | 20 | 20 | 0.6236 | 0.8910 | 0.5354 | 0.6544 |  |  | 0.4870 | 0.4346 |
| Q14012 | 17 | 523 | 0.7404 | 0.7714 | 1.0000 | 0.7399 |  |  | 0.5000 | 0.7083 |
| O95819 | 277 | 509 | 0.6268 | 0.8017 | 0.6480 | 0.7341 | 0.5154 | 0.7527 | 0.5534 | 0.6698 |
| P29322 | 3 | 12 | 0.5313 | 0.7333 | 0.6250 | 0.8384 |  |  | 0.5000 | 0.6888 |
| Q56UN5 | 105 | 59 | 0.5256 | 0.5752 |  | 0.6213 |  |  | 0.5000 | 0.6556 |
| Q64617 | 54 | 44 |  |  |  |  |  |  |  |  |
| P45985 | 3 | 20 | 0.5350 | 0.8393 |  |  |  |  | 0.5000 | 0.6761 |
| P51812 | 158 | 625 |  |  | 0.5870 | 0.7071 | 0.5545 | 0.8419 |  |  |
| P53667 | 99 | 501 | 0.6042 | 0.8590 | 0.6250 | 0.6286 |  |  | 0.4992 | 0.7228 |
| O15197 | 3 | 1 | 0.5000 | 0.7826 |  |  |  |  | 0.5000 | 0.5887 |
| P06494 | 8 | 1 |  |  |  |  |  |  |  |  |
| P28482 | 59 | 488 |  |  | 0.4935 | 0.5033 | 0.5000 | 0.9751 | 0.5000 | 0.6969 |
| O15146 | 4 | 13 | 0.5769 | 0.8030 | 0.5351 | 0.5845 | 0.5000 | 0.7644 | 0.5000 | 0.8030 |
| Q16584 | 29 | 22 | 0.6000 | 0.7036 | 0.5704 | 0.7579 |  |  | 0.5000 | 0.6821 |
| P51813 | 9 | 17 | 0.5614 | 0.8235 | 0.6037 | 0.7531 | 0.5755 | 0.6339 | 0.5126 | 0.6854 |
| O43781 | 87 | 318 |  |  | 0.4968 | 0.8853 |  |  |  |  |
| O15075 | 9 | 465 | 0.5833 | 0.7611 |  |  |  |  | 0.5000 | 0.5866 |
| O95835 | 3 | 13 | 0.7409 | 0.7833 |  |  |  |  | 0.5000 | 0.7511 |
| Q9Y2U5 | 2 | 2 | 0.5396 | 0.8163 | 0.5128 | 0.7333 |  |  | 0.5933 | 0.7274 |
| Q8N568 | 2 | 14 | 0.5833 | 0.7061 | 0.7500 | 0.8062 |  |  | 0.5000 | 0.6389 |
| O75582 | 76 | 269 |  |  | 0.4967 | 0.7078 | 0.5346 | 0.9531 |  |  |
| Q96PF2 | 25 | 363 |  |  | 0.4969 | 0.6359 | 0.4972 | 0.7451 |  |  |
| P08581 | 92 | 616 | 0.5385 | 0.8167 | 0.6667 | 0.6043 | 0.5000 | 0.9044 | 0.5000 | 0.7316 |
| Q02111 | 1 | 0 |  |  |  |  |  |  |  |  |
| P29376 | 90 | 201 | 0.6659 | 0.8429 | 0.6359 | 0.6530 | 0.8095 | 0.8747 | 0.5395 | 0.6173 |
| P17252 | 258 | 540 |  |  | 0.7966 | 0.5439 | 0.4722 | 0.9190 |  |  |
| P15208 | 1 | 42 |  |  |  |  |  |  |  |  |
| Q13464 | 456 | 651 | 0.5621 | 0.7222 | 0.7072 | 0.7974 | 0.7167 | 0.9296 | 0.6496 | 0.7574 |
| Q9NY57 | 1 | 15 | 0.6667 | 1.0000 |  |  |  |  | 0.5000 | 0.4785 |
| Q14289 | 80 | 304 | 0.6563 | 0.7867 | 0.6364 | 0.7247 | 0.4940 | 0.8956 | 0.5368 | 0.7468 |
| P49185 | 3 | 3 |  |  |  |  |  |  |  |  |
| Q13188 | 155 | 471 | 0.5998 | 0.6905 | 0.5830 | 0.7719 | 0.4868 | 0.8367 | 0.5308 | 0.6033 |
| Q08345 | 8 | 10 | 0.5257 | 0.7407 |  |  |  |  | 0.5695 | 0.5847 |
| Q96KB5 | 22 | 425 |  |  | 0.5000 | 0.6128 |  |  |  |  |
| P25098 | 2 | 6 |  |  |  | 0.6012 |  |  | 0.5000 | 0.5998 |
| P09216 | 60 | 46 |  |  |  |  |  |  |  |  |
| P10721 | 385 | 508 | 0.6146 | 0.8308 | 0.4876 | 0.7054 | 0.5761 | 0.6604 | 0.5538 | 0.7359 |
| Q00535 | 399 | 974 | 0.7283 | 1.0000 | 0.7188 | 0.7388 | 0.5341 | 0.9400 | 0.5800 | 0.5770 |
| P29323 | 5 | 46 | 0.5000 | 0.7524 | 0.5000 | 0.5572 | 0.4985 | 0.7655 | 0.5000 | 0.5324 |
| Q86UX6 | 1 | 15 | 0.7500 | 1.0000 |  |  |  |  | 0.5000 | 0.4613 |
| P51955 | 84 | 665 | 0.5000 | 0.7400 | 0.5000 | 0.5940 | 0.7486 | 0.9157 | 0.5000 | 0.6857 |
| Q15746 | 24 | 33 | 0.5603 | 0.7385 | 0.6538 | 0.6980 |  |  | 0.5000 | 0.7535 |
| P45983 | 397 | 936 | 0.6185 | 0.5667 | 0.9932 | 0.6456 |  |  | 0.5934 | 0.6071 |
| O14976 | 9 | 9 | 0.4762 | 0.7822 |  |  |  |  | 0.5372 | 0.6246 |
| Q02763 | 337 | 245 | 0.6809 | 0.6967 | 0.6119 | 0.6566 | 0.8534 | 0.8249 | 0.6773 | 0.7261 |
| Q86YV6 | 3 | 13 | 0.5833 | 0.6212 |  |  |  |  | 0.5000 | 0.7512 |
| Q9NWZ3 | 130 | 546 | 0.6560 | 0.7393 | 0.6840 | 0.8403 |  |  | 0.5162 | 0.8225 |
| Q15375 | 4 | 12 | 0.5356 | 0.6706 | 0.6635 | 0.5911 |  |  | 0.5000 | 0.6937 |
| Q13873 | 1 | 16 | 0.5000 | 0.5079 |  |  |  |  | 0.5000 | 0.6057 |
| P22607 | 107 | 476 | 0.6693 | 0.9375 | 0.6464 | 0.7637 | 0.5000 | 0.6384 | 0.5502 | 0.7006 |
| Q9BQI3 | 14 | 6 | 0.5000 | 0.3934 |  |  |  |  | 0.5000 | 0.5298 |
| P05696 | 74 | 46 |  |  |  |  |  |  |  |  |
| Q16512 | 3 | 16 | 0.5909 | 0.8690 | 0.5882 | 0.7524 |  |  | 0.5000 | 0.6568 |
| P05622 | 110 | 316 |  |  |  |  |  |  |  |  |
| P42685 | 124 | 265 | 0.6595 | 0.8889 | 0.6465 | 0.7712 | 0.7180 | 0.7758 | 0.6360 | 0.7814 |
| Q09013 | 2 | 20 | 0.5527 | 0.8423 | 0.9969 | 0.9260 |  |  | 0.5000 | 0.6386 |
| P18266 | 1 | 2 |  |  |  |  |  |  |  |  |
| Q8IU85 | 35 | 258 | 0.6667 | 0.7333 | 0.7500 | 0.5073 | 0.5000 | 0.7723 | 0.5000 | 0.7424 |
| Q9UM73 | 167 | 551 | 0.7273 | 0.8472 | 0.6076 | 0.7958 | 0.8824 | 0.9447 | 0.5468 | 0.6136 |
| P54764 | 4 | 16 | 0.5500 | 0.7941 | 0.5714 | 0.7586 | 0.5167 | 0.6982 | 0.5000 | 0.6130 |
| Q14680 | 121 | 323 | 0.6000 | 0.7155 | 0.5500 | 0.6196 | 0.4910 | 0.7410 | 0.5179 | 0.7681 |
| Q9NRP7 | 2 | 14 | 0.5000 | 0.7053 |  |  |  |  | 0.5000 | 0.4567 |
| P16092 | 12 | 24 |  |  |  |  |  |  |  |  |
| P35918 | 107 | 92 |  |  |  |  |  |  |  |  |
| Q4JIM5 | 1 | 1 |  |  |  |  |  |  |  |  |
| P36897 | 202 | 136 | 0.3750 | 0.4000 |  | 0.9704 |  |  | 0.6234 | 0.7091 |
| Q05513 | 95 | 854 |  |  | 0.9896 | 0.8000 |  |  |  |  |
| P31750 | 1 | 4 |  |  |  |  |  |  |  |  |
| P54756 | 4 | 14 | 0.5556 | 0.8294 | 0.6000 | 0.7857 |  |  | 0.5000 | 0.6306 |
| Q03142 | 8 | 13 |  |  |  |  |  |  |  |  |
| P43403 | 60 | 109 | 0.6576 | 0.7778 | 0.9968 | 0.6626 |  |  | 0.4968 | 0.6217 |
| Q16288 | 151 | 402 | 0.6647 | 0.8519 | 0.6162 | 0.7002 | 0.6578 | 0.8922 | 0.5350 | 0.7277 |
| P00521 | 1 | 39 |  |  |  |  |  |  |  |  |

a A null value indicates that the kinase is not in the dataset.

# 4 Case study

Supplementary figure 3 summarizes the predicted and experiment kinase activity and selectivity profile of the case. The experiment validation was carried out by using the Eurofins’ KinaseProfiler Service (https://www.eurofinsdiscoveryservices.com/cms/cms-content/services/in-vitro-assays/kinases/kinase-profiler/). The percent activity of NVP-BHG712 was tested against a panel of 405 kinases, among which 282 fall in our MTDNN capacity panel (391 kinases). Filter-binding radiometric kinase activity assays were performed at a concentration of 1 μM, with the active threshold defined as 50%. Also, most of the novel “off-target” activities have been confirmed by subsequent experiments at lower compound concentrations (0.1 μM and 0.01 μM). The results are shown in supplementary table 3. According to the results at 1 μM, the model shows auROC of 0.86, recall of 0.69, precision of 0.41 and balanced accuracy of 0.80.

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### Supplementary figure 3. Kinome map and selectivity of the predicted and experimental bioactivities of NVP-BHG712. (A) Kinases coloured in red have predicted active probability>0.5 (B) Kinases coloured in red have experimental %activity<50% at 1 μM. (C, D) Standard score, gini score and bar plots of predicted and experimental group selectivity. When a group has an odds ratio significantly greater than 1, the bar is coloured red (right). (E) Chemical depiction and cross references of NVP-BHG712. ‘\*’: 0.01<p<0.05; ‘\*\*’: 0.001<p<0.01; ‘\*\*\*’: p<0.001.

### Supplementary table 3. The predicted activity probability and experimental %activity of NVP-BHG712.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| UniProt ID | Kinase | Predicted  probability | at 1 µMa | at 0.1 µMb | at 0.01 µMc |
| Q2M2I8 | AAK1(h) | 0.0144 | 96 |  |  |
| P00519 | Abl(h) | 0.9481 | 24 | 74 | 101 |
| P00520 | Abl(m) | 0.7683 | 3 | 24 | 78 |
| Q07912 | ACK1(h) | 0.4318 | 91 |  |  |
| Q9UM73 | ALK(h) | 0.3388 | 107 |  |  |
| P37023 | ALK1(h) | 0.0892 | 103 |  |  |
| Q04771 | ALK2(h) | 0.1853 | 104 |  |  |
| P36896 | ALK4(h) | 0.132 | 106 |  |  |
| P42684 | Arg(h) | 0.8972 | 18 | 38 | 84 |
| Q13131 | AMPKα1(h) | 0.001 | 99 |  |  |
| P54646 | AMPKα2(h) | 0.0175 | 105 |  |  |
| Q4JIM5 | Arg(m) | 0.5884 | 20 | 42 | 84 |
| O60285 | ARK5(h) | 0.0528 | 113 |  |  |
| Q99683 | ASK1(h) | 0.0004 | 99 |  |  |
| O14965 | Aurora-A(h) | 0.0284 | 102 |  |  |
| Q96GD4 | Aurora-B(h) | 0.0662 | 105 |  |  |
| Q9UQB9 | Aurora-C(h) | 0.4904 | 130 |  |  |
| P30530 | Axl(h) | 0.9661 | 94 |  |  |
| P51451 | Blk(h) | 0.9612 | 56 |  |  |
| P16277 | Blk(m) | 0.8402 | 52 |  |  |
| Q13873 | BMPR2(h) | 0.007 | 79 |  |  |
| P51813 | Bmx(h) | 0.8825 | 100 |  |  |
| Q13882 | BRK(h) | 0.9143 | 113 |  |  |
| Q8TDC3 | BrSK1(h) | 0 | 109 |  |  |
| Q06187 | BTK(h) | 0.7414 | 91 |  |  |
| P15056 | B-Raf(h) | 0.8461 | 41 |  |  |
| Q14012 | CaMKI(h) | 0 | 115 |  |  |
| Q96NX5 | CaMKIγ(h) | 0.0115 | 109 |  |  |
| Q9UQM7 | CaMKIIα(h) | 0 | 100 |  |  |
| Q13554 | CaMKIIβ(h) | 0 | 107 |  |  |
| Q13555 | CaMKIIγ(h) | 0.0001 | 103 |  |  |
| Q13557 | CaMKIIδ(h) | 0 | 108 |  |  |
| Q16566 | CaMKIV(h) | 0.0008 | 110 |  |  |
| Q8N5S9 | CaMKK1(h) | 0.0104 | 97 |  |  |
| Q96RR4 | CaMKK2(h) | 0.0018 | 98 |  |  |
| O00311 | Cdc7/cyclinB1(h) | 0.0032 | 106 |  |  |
| P06493 | CDK1/cyclinB(h) | 0.0027 | 106 |  |  |
| P24941 | CDK2/cyclinA(h) | 0.0002 | 103 |  |  |
| Q00526 | CDK3/cyclinE(h) | 0.0013 | 99 |  |  |
| P11802 | CDK4/cyclinD3(h) | 0.0057 | 101 |  |  |
| Q00535 | CDK5/p35(h) | 0.0001 | 61 |  |  |
| Q00534 | CDK6/cyclinD3(h) | 0.0126 | 108 |  |  |
| P50613 | CDK7/cyclinH/MAT1(h) | 0.0067 | 111 |  |  |
| P50750 | CDK9/cyclin T1(h) | 0.0012 | 105 |  |  |
| Q00536 | CDK16/cyclinY(h) | 0.0125 | 133 |  |  |
| Q92772 | CDKL2(h) | 0.4845 | 92 |  |  |
| Q8IVW4 | CDKL3(h) | 0.4771 | 67 |  |  |
| O14757 | CHK1(h) | 0.0001 | 107 |  |  |
| O96017 | CHK2(h) | 0.0005 | 99 |  |  |
| Q9HCP0 | CK1γ1(h) | 0.0039 | 110 |  |  |
| P78368 | CK1γ2(h) | 0.0003 | 123 |  |  |
| Q9Y6M4 | CK1γ3(h) | 0.0001 | 110 |  |  |
| P48730 | CK1δ(h) | 0.025 | 102 |  |  |
| P68400 | CK2α1(h) | 0.0545 | 101 |  |  |
| P19784 | CK2α2(h) | 0.0008 | 74 |  |  |
| Q8TDR2 | CLIK1(h) | 0.0526 | 100 |  |  |
| P49759 | CLK1(h) | 0.0574 | 84 |  |  |
| P49760 | CLK2(h) | 0.0619 | 111 |  |  |
| P49761 | CLK3(h) | 0 | 93 |  |  |
| Q9HAZ1 | CLK4(h) | 0.0925 | 114 |  |  |
| P10721 | cKit(h) | 0.9812 | 73 |  |  |
| O14578 | CRIK(h) | 0.0035 | 111 |  |  |
| P41240 | CSK(h) | 0.0628 | 95 |  |  |
| P04049 | c-RAF(h) | 0.4611 | 20 | 88 | 101 |
| P12931 | cSRC(h) | 0.7868 | 55 |  |  |
| P53355 | DAPK1(h) | 0.0083 | 103 |  |  |
| Q9UIK4 | DAPK2(h) | 0.012 | 109 |  |  |
| Q8N568 | DCAMKL2(h) | 0.0034 | 124 |  |  |
| Q9C098 | DCAMKL3(h) | 0.0138 | 119 |  |  |
| Q08345 | DDR1(h) | 0.5981 | 7 | 16 | 62 |
| Q09013 | DMPK(h) | 0.0032 | 119 |  |  |
| Q9UEE5 | DRAK1(h) | 0.0016 | 132 |  |  |
| O94768 | DRAK2(h) | 0.0596 | 107 |  |  |
| Q13627 | DYRK1A(h) | 0.0018 | 86 |  |  |
| Q9Y463 | DYRK1B(h) | 0.0004 | 83 |  |  |
| Q92630 | DYRK2(h) | 0.0949 | 106 |  |  |
| O43781 | DYRK3(h) | 0.5077 | 92 |  |  |
| O00418 | eEF-2K(h) | 0 | 115 |  |  |
| P00533 | EGFR(h) | 0.0775 | 119 |  |  |
| P21709 | EphA1(h) | 0.4293 | 48 |  |  |
| P29317 | EphA2(h) | 0.9787 | 10 | 70 | 95 |
| P29320 | EphA3(h) | 0.799 | 29 | 76 | 95 |
| P54764 | EphA4(h) | 0.2989 | 75 |  |  |
| P54756 | EphA5(h) | 0.2207 | 16 | 70 | 82 |
| Q15375 | EphA7(h) | 0.0436 | 72 |  |  |
| P29322 | EphA8(h) | 0.3938 | 4 | 34 | 82 |
| P29323 | EphB2(h) | 0.7001 | 27 | 83 | 89 |
| P54762 | EphB1(h) | 0.6729 | 16 | 76 | 97 |
| P54753 | EphB3(h) | 0.3828 | 73 |  |  |
| P54760 | EphB4(h) | 0.7188 | 80 |  |  |
| P04626 | ErbB2(h) | 0.3311 | 106 |  |  |
| Q15303 | ErbB4(h) | 0.0253 | 103 |  |  |
| Q05397 | FAK(h) | 0.8715 | 102 |  |  |
| P16591 | Fer(h) | 0.2319 | 101 |  |  |
| P07332 | Fes(h) | 0.0825 | 112 |  |  |
| P11362 | FGFR1(h) | 0.1392 | 89 |  |  |
| P21802 | FGFR2(h) | 0.6829 | 100 |  |  |
| P22607 | FGFR3(h) | 0.0779 | 112 |  |  |
| P22455 | FGFR4(h) | 0.2702 | 103 |  |  |
| P09769 | Fgr(h) | 0.8342 | 70 |  |  |
| P17948 | Flt1(h) | 0.3051 | 40 |  |  |
| P36888 | Flt3(h) | 0.2694 | 82 |  |  |
| P35916 | Flt4(h) | 0.7016 | 36 |  |  |
| P07333 | Fms(h) | 0.9658 | 31 |  |  |
| P06241 | Fyn(h) | 0.9093 | 74 |  |  |
| Q12851 | GCK(h) | 0.11 | 100 |  |  |
| Q15835 | GRK1(h) | 0.2947 | 88 |  |  |
| P25098 | GRK2(h) | 0.0532 | 103 |  |  |
| P34947 | GRK5(h) | 0.0002 | 120 |  |  |
| Q8WTQ7 | GRK7(h) | 0.1159 | 95 |  |  |
| P49840 | GSK3α(h) | 0.0319 | 90 |  |  |
| P49841 | GSK3β(h) | 0.032 | 103 |  |  |
| P08631 | Hck(h) | 0.9022 | 9 | 56 | 100 |
| Q86Z02 | HIPK1(h) | 0.0174 | 89 |  |  |
| Q9H2X6 | HIPK2(h) | 0.7418 | 110 |  |  |
| Q9H422 | HIPK3(h) | 0.6714 | 95 |  |  |
| Q8NE63 | HIPK4(h) | 0.293 | 131 |  |  |
| Q92918 | HPK1(h) | 0.2461 | 99 |  |  |
| Q9BQI3 | HRI(h) | 0.9989 | 117 |  |  |
| Q9UPZ9 | ICK(h) | 0.1483 | 111 |  |  |
| P08069 | IGF-1R(h) | 0.051 | 119 |  |  |
| O15111 | IKKα(h) | 0 | 112 |  |  |
| O14920 | IKKβ(h) | 0.0166 | 88 |  |  |
| Q14164 | IKKε(h) | 0.0022 | 105 |  |  |
| P06213 | IR(h) | 0.0041 | 106 |  |  |
| Q8IVH8 | IRE1(h) | 0.2886 | 100 |  |  |
| P14616 | IRR(h) | 0.0131 | 96 |  |  |
| P51617 | IRAK1(h) | 0.002 | 120 |  |  |
| Q9NWZ3 | IRAK4(h) | 0.0003 | 78 |  |  |
| Q08881 | Itk(h) | 0.0202 | 98 |  |  |
| O60674 | JAK2(h) | 0.1223 | 107 |  |  |
| P52333 | JAK3(h) | 0.0472 | 83 |  |  |
| P45983 | JNK1α1(h) | 0.0001 | 103 |  |  |
| P45984 | JNK2α2(h) | 0.0258 | 90 |  |  |
| P53779 | JNK3(h) | 0.0035 | 82 |  |  |
| P35968 | KDR(h) | 0.0799 | 63 |  |  |
| P06239 | Lck(h) | 0.9918 | 10 | 54 | 98 |
| P53667 | LIMK1(h) | 0.2785 | 98 |  |  |
| P53671 | LIMK2(h) | 0.8672 | 92 |  |  |
| Q15831 | LKB1(h) | 0.0164 | 96 |  |  |
| O94804 | LOK(h) | 0.0198 | 107 |  |  |
| P07948 | Lyn(h) | 0.9901 | 2 | 22 | 73 |
| Q5S007 | LRRK2(h) | 0.0064 | 114 |  |  |
| P29376 | LTK(h) | 0.2336 | 114 |  |  |
| P28482 | MAPK1(h) | 0 | 96 |  |  |
| O95819 | MAP4K4(h) | 0.1237 | 102 |  |  |
| Q9Y4K4 | MAP4K5(h) | 0.6743 | 97 |  |  |
| P49137 | MAPKAP-K2(h) | 0.0006 | 106 |  |  |
| Q16644 | MAPKAP-K3(h) | 0 | 114 |  |  |
| Q02750 | MEK1(h) | 0.0982 | 101 |  |  |
| P36507 | MEK2(h) | 0.0218 | 107 |  |  |
| Q9P0L2 | MARK1(h) | 0.0025 | 85 |  |  |
| P27448 | MARK3(h) | 0.0058 | 107 |  |  |
| Q96L34 | MARK4(h) | 0.0023 | 99 |  |  |
| Q9Y2U5 | MEKK2(h) | 0.1219 | 112 |  |  |
| Q99759 | MEKK3(h) | 0.0641 | 100 |  |  |
| Q14680 | MELK(h) | 0.2288 | 82 |  |  |
| P08581 | Met(h) | 0.0155 | 127 |  |  |
| Q8N4C8 | MINK(h) | 0.218 | 100 |  |  |
| P46734 | MKK3(h) | 0.0027 | 65 |  |  |
| P52564 | MKK6(h) | 0.0015 | 86 |  |  |
| Q15746 | MLCK(h) | 0.0387 | 101 |  |  |
| P80192 | MLK1(h) | 0.0019 | 103 |  |  |
| Q02779 | MLK2(h) | 0.0007 | 90 |  |  |
| Q16584 | MLK3(h) | 0.0033 | 93 |  |  |
| Q9HBH9 | Mnk2(h) | 0.0023 | 82 |  |  |
| Q5VT25 | MRCKα(h) | 0.0002 | 111 |  |  |
| Q9Y5S2 | MRCKβ(h) | 0.004 | 110 |  |  |
| O75582 | MSK1(h) | 0.0067 | 125 |  |  |
| O75676 | MSK2(h) | 0.0663 | 123 |  |  |
| Q9UPE1 | MSSK1(h) | 0.0845 | 130 |  |  |
| Q13043 | MST1(h) | 0.0454 | 103 |  |  |
| Q13188 | MST2(h) | 0.1691 | 91 |  |  |
| Q9Y6E0 | MST3(h) | 0.0157 | 112 |  |  |
| Q9P289 | MST4(h) | 0.0045 | 98 |  |  |
| O15146 | MuSK(h) | 0.1505 | 87 |  |  |
| Q9H1R3 | MYLK2(h) | 0.014 | 93 |  |  |
| Q8WXR4 | MYO3B(h) | 0.0036 | 100 |  |  |
| Q9Y2H1 | NDR2(h) | 0.0179 | 101 |  |  |
| Q96PY6 | NEK1(h) | 0.0007 | 125 |  |  |
| P51955 | NEK2(h) | 0.013 | 105 |  |  |
| P51957 | NEK4(h) | 0.0014 | 99 |  |  |
| Q9HC98 | NEK6(h) | 0.0258 | 104 |  |  |
| Q8TDX7 | NEK7(h) | 0.0014 | 103 |  |  |
| Q8IY84 | NIM1(h) | 0.023 | 106 |  |  |
| Q9UBE8 | NLK(h) | 0.5973 | 101 |  |  |
| Q9H093 | NUAK2(h) | 0.0152 | 102 |  |  |
| P23443 | p70S6K(h) | 0.1042 | 104 |  |  |
| Q13153 | PAK1(h) | 0.0001 | 107 |  |  |
| Q13177 | PAK2(h) | 0.0004 | 98 |  |  |
| O96013 | PAK4(h) | 0.001 | 101 |  |  |
| O75914 | PAK3(h) | 0.0016 | 102 |  |  |
| Q9P286 | PAK5(h) | 0.0182 | 95 |  |  |
| Q9NQU5 | PAK6(h) | 0.0045 | 101 |  |  |
| Q7KZI7 | PAR-1Bα(h) | 0.0022 | 104 |  |  |
| Q96RG2 | PASK(h) | 0.0006 | 109 |  |  |
| Q9NZJ5 | PEK(h) | 0.0245 | 103 |  |  |
| P16234 | PDGFRα(h) | 0.9889 | 86 |  |  |
| P09619 | PDGFRβ(h) | 0.9702 | 104 |  |  |
| Q16816 | PhKγ1(h) | 0.0001 | 112 |  |  |
| P15735 | PhKγ2(h) | 0 | 1 | 78 | 79 |
| P11309 | Pim-1(h) | 0.0572 | 69 |  |  |
| Q9P1W9 | Pim-2(h) | 0.0009 | 121 |  |  |
| Q86V86 | Pim-3(h) | 0.016 | 118 |  |  |
| P17612 | PKA(h) | 0 | 110 |  |  |
| P22694 | PKAcβ(h) | 0 | 125 |  |  |
| P31749 | PKBα(h) | 0.0002 | 90 |  |  |
| P31751 | PKBβ(h) | 0 | 141 |  |  |
| Q9Y243 | PKBγ(h) | 0 | 111 |  |  |
| P17252 | PKCα(h) | 0.0007 | 101 |  |  |
| P05771 | PKCβII(h) | 0.0021 | 109 |  |  |
| P05129 | PKCγ(h) | 0.0001 | 112 |  |  |
| Q05655 | PKCδ(h) | 0 | 99 |  |  |
| Q02156 | PKCη(h) | 0.0009 | 98 |  |  |
| P41743 | PKCι(h) | 0 | 106 |  |  |
| Q15139 | PKCμ(h) | 0.0004 | 115 |  |  |
| Q04759 | PKCθ(h) | 0.001 | 97 |  |  |
| Q05513 | PKCζ(h) | 0 | 100 |  |  |
| Q9BZL6 | PKD2(h) | 0.0002 | 105 |  |  |
| O94806 | PKD3(h) | 0.0056 | 100 |  |  |
| Q13976 | PKG1α(h) | 0.0002 | 2 | 97 | 81 |
| P19525 | PKR(h) | 0.0159 | 113 |  |  |
| P53350 | Plk1(h) | 0.0055 | 101 |  |  |
| Q9H4B4 | Plk3(h) | 0.0031 | 107 |  |  |
| O00444 | Plk4(h) | 0.1022 | 101 |  |  |
| Q8IW41 | PRAK(h) | 0.0024 | 91 |  |  |
| Q13237 | PRKG2(h) | 0 | 98 |  |  |
| Q16512 | PRK1(h) | 0.0094 | 95 |  |  |
| Q16513 | PRK2(h) | 0 | 85 |  |  |
| P51817 | PrKX(h) | 0.0007 | 103 |  |  |
| P42685 | PTK5(h) | 0.9998 | 3 | 13 | 71 |
| Q14289 | Pyk2(h) | 0.2498 | 106 |  |  |
| P07949 | Ret(h) | 0.9553 | 99 |  |  |
| Q13546 | RIPK1(h) | 0.0123 | 96 |  |  |
| O43353 | RIPK2(h) | 0.0901 | 89 |  |  |
| Q13464 | ROCK-I(h) | 0.0011 | 110 |  |  |
| O75116 | ROCK-II(h) | 0.015 | 102 |  |  |
| Q04912 | Ron(h) | 0.1767 | 117 |  |  |
| P08922 | Ros(h) | 0.085 | 98 |  |  |
| Q06418 | Rse(h) | 0.3247 | 108 |  |  |
| P51812 | Rsk2(h) | 0.0966 | 113 |  |  |
| Q16539 | SAPK2a(h) | 0.9933 | 73 |  |  |
| P53778 | SAPK3(h) | 0.0811 | 100 |  |  |
| O15264 | SAPK4(h) | 0.2489 | 109 |  |  |
| O00141 | SGK(h) | 0 | 112 |  |  |
| P57059 | SIK(h) | 0.3477 | 145 |  |  |
| Q9H0K1 | SIK2(h) | 0.1099 | 105 |  |  |
| Q9Y2K2 | SIK3(h) | 0.1037 | 116 |  |  |
| Q9H2G2 | SLK(h) | 0.0848 | 104 |  |  |
| Q9NYY3 | Snk(h) | 0.0013 | 111 |  |  |
| P12931 | Src(1-530)(h) | 0.7868 | 56 |  |  |
| Q9H3Y6 | SRMS(h) | 0.575 | 78 |  |  |
| Q96SB4 | SRPK1(h) | 0.0005 | 101 |  |  |
| O75716 | STK16(h) | 0.0157 | 110 |  |  |
| O00506 | STK25(h) | 0.0161 | 107 |  |  |
| Q9NY57 | STK32B(h) | 0.0021 | 96 |  |  |
| Q86UX6 | STK32C(h) | 0.0023 | 95 |  |  |
| Q9BYT3 | STK33(h) | 0.012 | 100 |  |  |
| P43405 | Syk(h) | 0.1284 | 92 |  |  |
| Q7L7X3 | TAO1(h) | 0.1803 | 99 |  |  |
| Q9H2K8 | TAO3(h) | 0.1122 | 87 |  |  |
| Q9UHD2 | TBK1(h) | 0.0002 | 104 |  |  |
| P36897 | TGFBR1(h) | 0.4827 | 100 |  |  |
| Q9UKI8 | TLK1(h) | 0.019 | 99 |  |  |
| Q86UE8 | TLK2(h) | 0.0109 | 103 |  |  |
| Q9UKE5 | TNIK(h) | 0.0157 | 115 |  |  |
| P04629 | TrkA(h) | 0.09 | 61 |  |  |
| Q16620 | TrkB(h) | 0.6186 | 62 |  |  |
| Q16288 | TrkC(h) | 0.5894 | 32 |  |  |
| Q9BXA7 | TSSK1(h) | 0 | 103 |  |  |
| Q96PF2 | TSSK2(h) | 0.0001 | 97 |  |  |
| P33981 | TTK(h) | 0.0078 | 96 |  |  |
| P42681 | Txk(h) | 0.2769 | 63 |  |  |
| P29597 | TYK2(h) | 0.0006 | 104 |  |  |
| O75385 | ULK1(h) | 0.1459 | 99 |  |  |
| Q8IYT8 | ULK2(h) | 0.1438 | 111 |  |  |
| Q6PHR2 | ULK3(h) | 0.149 | 107 |  |  |
| P30291 | Wee1(h) | 0.0049 | 94 |  |  |
| P07947 | Yes(h) | 0.6238 | 37 |  |  |
| Q9NYL2 | ZAK(h) | 0.2295 | 9 | 67 | 108 |
| P43403 | ZAP-70(h) | 0.0002 | 120 |  |  |
| O43293 | ZIPK(h) | 0.0421 | 113 |  |  |

a, b, c The %activities of a kinase at NVP-BHG712 concentrations of 1 μM, 0.1 μM and 0.01 μM. A null value indicates that the activity was not tested.

# 5 Computational methods

Multitask deep Neural network models were developed with Tensorflow (Version 1.6.0) and DeepChem (Version 2.1.0). All trainings are performed on standard NVIDIA GPUs. The code is written with Python 3.6.

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