**Supplementary Materials**

**Appendix 1**

**Table S1**: Top 50 drug-pathway associations that were predicted by GIP.

|  |  |
| --- | --- |
| **Pathway ID (hsa00)** | **Drug ID(KEGG)** |
| 4010 | D06407 |
| 4060 | D09689 |
| 4080  4010  4370  4270  4020  240  4012  4060  4060  140  4510  4012  4020  5212  4510  4370  4370  4010  5110  983  4020  4012  4370  4370  4730  4060  4370  4110  4020  230  4370  4060  4060  4010  4110  4370  3320  4610  4060  4010  4510  4920  4012  4060  4010  4370  4010  4370  4150 | D00371  D09883  D09589  D00227  D09635  D05400  D01441  D09883  D09690  D00075  D10224  D08066  D08907  D04023  D10190  D01441  D10465  D04025  D08369  D07974  D08883  D10405  D08907  D10064  D08369  D08279  D03350  D10441  D08881  D01846  D09010  D03736  D10202  D09683  D08066  D09690  D04050  D00138  D10175  D05819  D09903  D04050  D09920  D10064  D08369  D00752  D10202  D04023  D00107 |

**Table S2**: Top 50 drug-pathway associations that were predicted by GBSSL.

|  |  |
| --- | --- |
| **Pathway ID (hsa00)** | **Drug ID(KEGG)** |
| 4080 | D00371 |
| 4370 | D10486 |
| 4060 | D09728 |
| 4060 | D03252 |
| 4270 | D00371 |
| 4010 | D09883 |
| 4270 | D00227 |
| 4510 | D10190 |
| 4370 | D10465 |
| 140 | D00075 |
| 4060 | D09883 |
| 4510 | D10224 |
| 4010 | D06407 |
| 4010 | D09618 |
| 670 | D03998 |
| 4060 | D09689 |
| 240 | D03998 |
| 4370 | D09919 |
| 4370 | D01977 |
| 4010 | D09683 |
| 4020 | D09618 |
| 4010 | D10190 |
| 4370 | D09920 |
| 4012 | D08881 |
| 4060 | D09690 |
| 4910 | D02042 |
| 4910 | D09786 |
| 5110 | D10222 |
| 5215 | D02008 |
| 4650  4370  4020  3320  3320  4020  4020  4370  4610  4020  4370  4270  5110  5110  4510  3320  4920  4370  4370  4610  4370 | D10078  D09589  D03898  D10019  D10319  D09635  D10190  D09883  D05834  D08881  D08656  D03898  D10431  D00944  D08552  D00126  D00126  D04498  D03350  D03978  D09010 |

**Table S3**: Top 50 drug-pathway associations that were predicted by BLM.

|  |  |
| --- | --- |
| **Pathway ID (hsa00)** | **Drug ID(KEGG)** |
| 982 | D05147 |
| 4080 | C01245 |
| 4080 | C00165 |
| 4012 | D05147 |
| 4080 | C00575 |
| 4610 | D05147 |
| 140 | D00075 |
| 4080 | D00371 |
| 4010 | D09883 |
| 480 | D00707 |
| 4930 | C05981 |
| 4270 | D00371 |
| 4060 | D10202 |
| 4060 | D09883 |
| 4510 | D05147 |
| 4520 | C05981 |
| 5211 | C05981 |
| 230 | C01245 |
| 5212 | C05981 |
| 4512 | C05981 |
| 240 | D00752 |
| 240 | D01206 |
| 240 | D02365 |
| 240 | D04936 |
| 240 | D05094 |
| 240 | D05095 |
| 4370 | D09010 |
| 670 | D01155 |
| 670 | D02368 |
| 670 | D10222 |
| 4020 | D03898 |
| 983 | D03378 |
| 983 | D03546 |
| 983 | D04245 |
| 4270 | D03898 |
| 240 | D03998 |
| 4010 | D09618 |
| 230 | D01846 |
| 983 | D06596 |
| 983 | D03828 |
| 983 | D06503 |
| 983 | D07472 |
| 4370 | D10486 |
| 983 | D10431 |
| 4110 | D05147 |
| 230 | D06102 |
| 4020 | D10202 |
| 4010 | D10202 |

**Appendix 2**

**Table S4**: the possible drug-pathway interactions that predicted by GIP and GBSSL methods

|  |  |
| --- | --- |
| Predicted Drug-pathway interaction | Drug structure |
| hsa004510  D10224s | http://www.genome.jp/Fig/drug/D10224.gif http://www.genome.jp/Fig/drug/D10465.gif |
| hsa004012  D08066s | http://www.genome.jp/Fig/drug/D08066.gif http://www.genome.jp/Fig/drug/D01441.gif |
| hsa004370  D10465s | http://www.genome.jp/Fig/drug/D10465.gif http://www.genome.jp/Fig/drug/D10224.gif |
| hsa00983  D07974s | http://www.genome.jp/Fig/drug/D07974.gif http://www.genome.jp/Fig/drug/D00584.gif |
| hsa04110  D08066 | http://www.genome.jp/Fig/drug/D08066.gifhttp://www.genome.jp/Fig/drug/D01441.gif |
| hsa04370  D09010s | http://www.genome.jp/Fig/drug/D09010.gif http://www.genome.jp/Fig/drug/D00330.gif |

Note: the left side in drug structure column is 2d-structure of drugs which were predicted to have association with pathways, and the right side is the 2d-structure of drugs which known to have associations with corresponding pathways.