

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	D00371
4010	D09883
4370	D09589
4270	D00227
4020	D09635
240	D05400
4012	D01441
4060	D09883
4060	D09690
140	D00075
4510	D10224
4012	D08066
4020	D08907
5212	D04023
4510	D10190
4370	D01441
4370	D10465
4010	D04025
5110	D08369
983	D07974
4020	D08883
4012	D10405
4370	D08907
4370	D10064
4730	D08369
4060	D08279
4370	D03350
4110	D10441
4020	D08881
230	D01846
4370	D09010
4060	D03736
4060	D10202

4010	D09683
4110	D08066
4370	D09690
3320	D04050
4610	D00138
4060	D10175
4010	D05819
4510	D09903
4920	D04050
4012	D09920
4060	D10064
4010	D08369
4370	D00752
4010	D10202
4370	D04023
4150	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	D10078
4370	D09589
4020	D03898
3320	D10019
3320	D10319
4020	D09635
4020	D10190
4370	D09883
4610	D05834
4020	D08881
4370	D08656
4270	D03898
5110	D10431
5110	D00944
4510	D08552
3320	D00126
4920	D00126
4370	D04498
4370	D03350
4610	D03978
4370	D09010

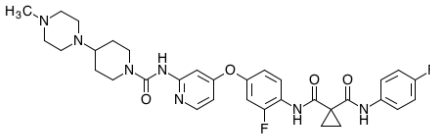
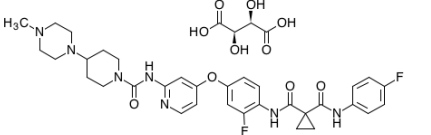
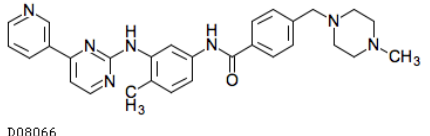
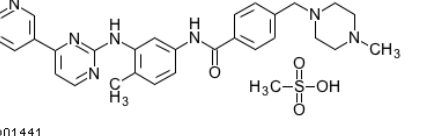
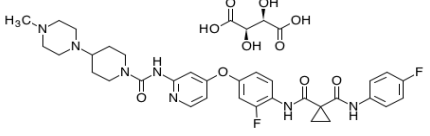
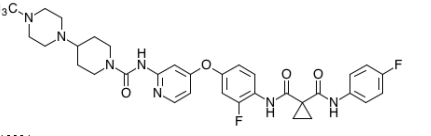
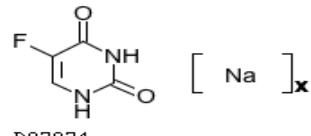
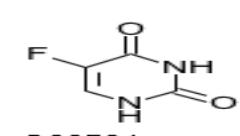
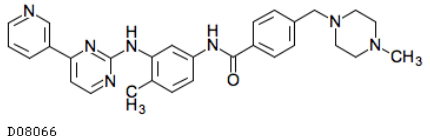
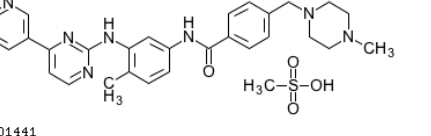
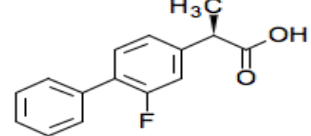
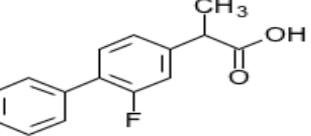
Table S3: Top 50 drug-pathway associations that were predicted by BLM.

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	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>D10224</p> </div> <div style="text-align: center;">  <p>D10465</p> </div> </div>
hsa004012 D08066s	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>D08066</p> </div> <div style="text-align: center;">  <p>D01441</p> </div> </div>
hsa004370 D10465s	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>D10465</p> </div> <div style="text-align: center;">  <p>D10224</p> </div> </div>
hsa00983 D07974s	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>D07974</p> </div> <div style="text-align: center;">  <p>D00584</p> </div> </div>
hsa04110 D08066	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>D08066</p> </div> <div style="text-align: center;">  <p>D01441</p> </div> </div>
hsa04370 D09010s	<div style="display: flex; justify-content: space-around;"> <div style="text-align: center;">  <p>D09010</p> </div> <div style="text-align: center;">  <p>D00330</p> </div> </div>

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.