

Table S3. Recall on the valid recommendation list length for all data sets with the network-based inference (NBI) method by 30 simulation times of 10-fold cross-validation test.

Datasets	Enzyme	Ion Channel	GPCRs	Nuclear Receptor	Approved	Global
Recall	0.935	0.981	0.948	0.851	0.741	0.736

Approved: data set of approved small molecular drugs in DrugBank, global: data set of approved and experimentally investigated small molecular drugs in DrugBank.