

Marina Boudin

❖ First lock: knowledge integration

Heterogeneous data

❖ DrugBank

❖ SIDER

❖ PharmGKB

❖ Human phenotype ontology (HPO)

❖ NPASS (natural compounds)

❖ Bio2RDF

 DRUGBANK

Pub  Chem

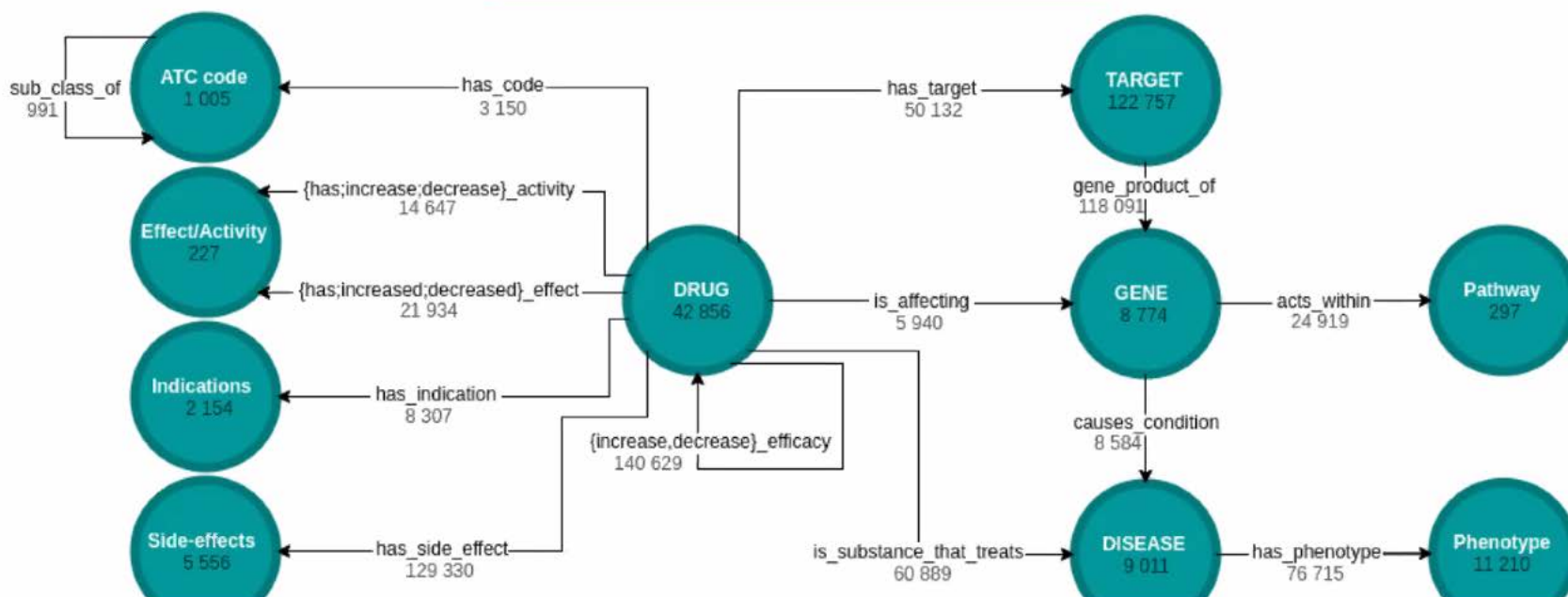
UniProt 



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Xiaodong LI (You) 12:12 AM

Another question, since the drug candidates need to be further verified in the lab, how to make sure that the scores obtained do help in the clinical trial. In other words, any suggestion to improve the confidence of the drugs to be recommended in addition to the score?

Marina Boudin 12:22 AM

We can look at the publications and clinical trials about those drugs. We can also use the structures of the drugs to compute the biological binding possibility of the link between the drug and the target. This technique allow us to reduce the scope of research to concentrate the investigations on leads that seems to have a great possibility to interact with precise targets.