

Systematic Drug Repositioning: Data and Informatics Showcase?

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Computational Biology, Quantitative Sciences
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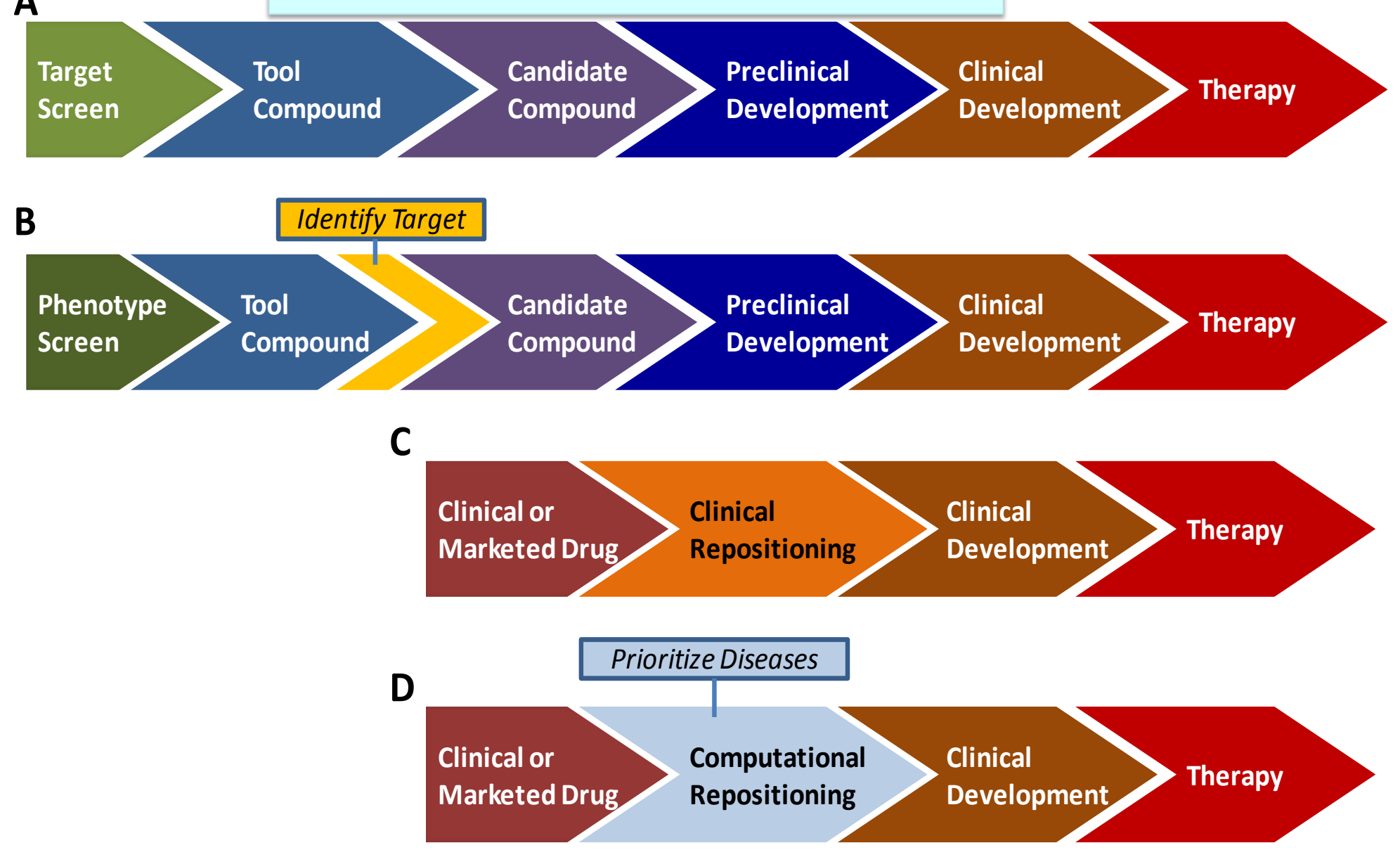
“The most fruitful basis for the discovery of a new drug is to start with an old drug.” ... Sir James Black

Repurposing

Drug repositioning or repurposing is the application of known drugs and compounds to new disease indications.

Drug	Original indication	New indication
Viagra	Hypertension	Erectile dysfunction
Wellbutrin	Depression	Smoking cessation
Minoxidil	Hypertension	Hair loss
Thalidomide	Antiemetic	Leprosy
AZT	Cancer?	AIDS

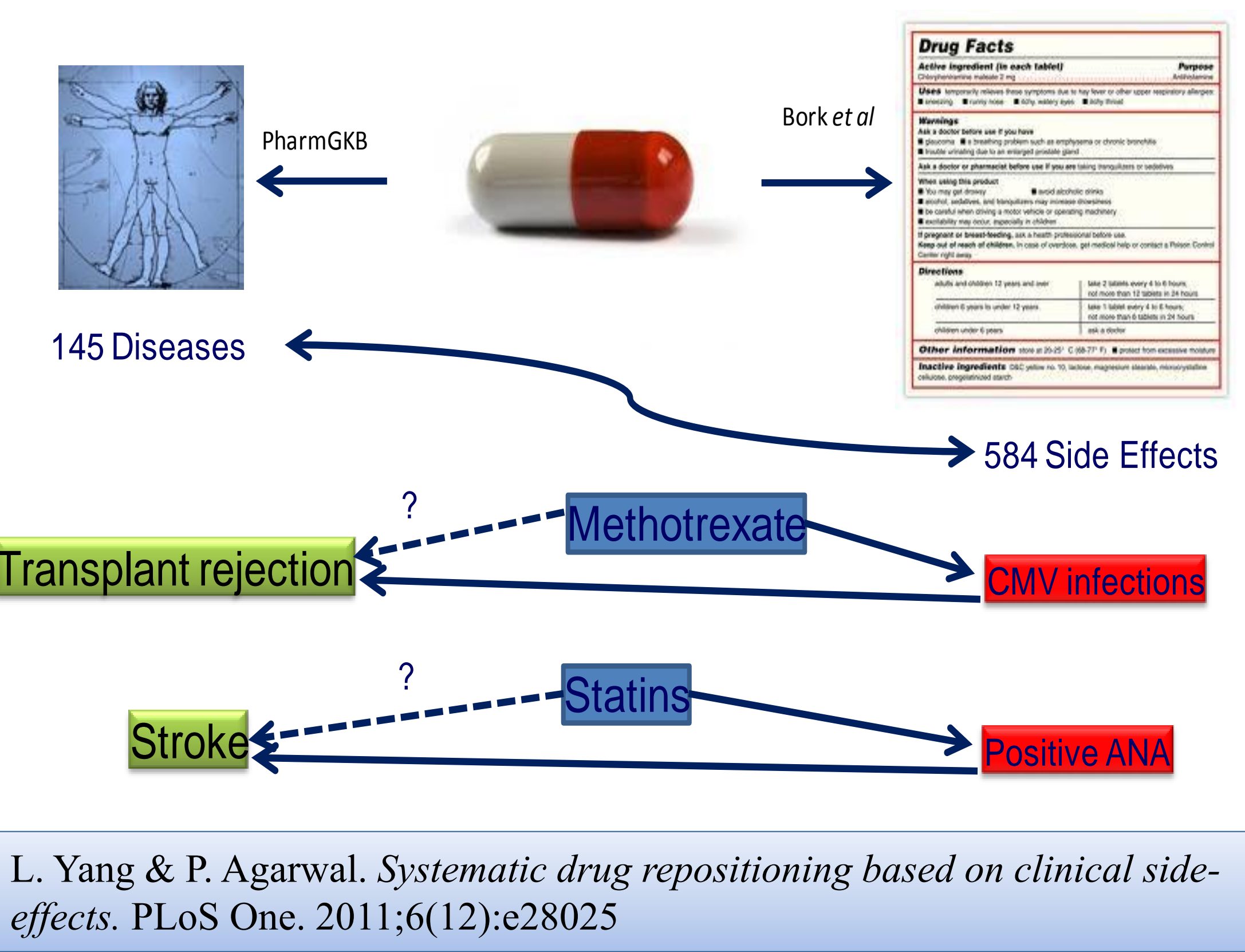
Shorter timelines



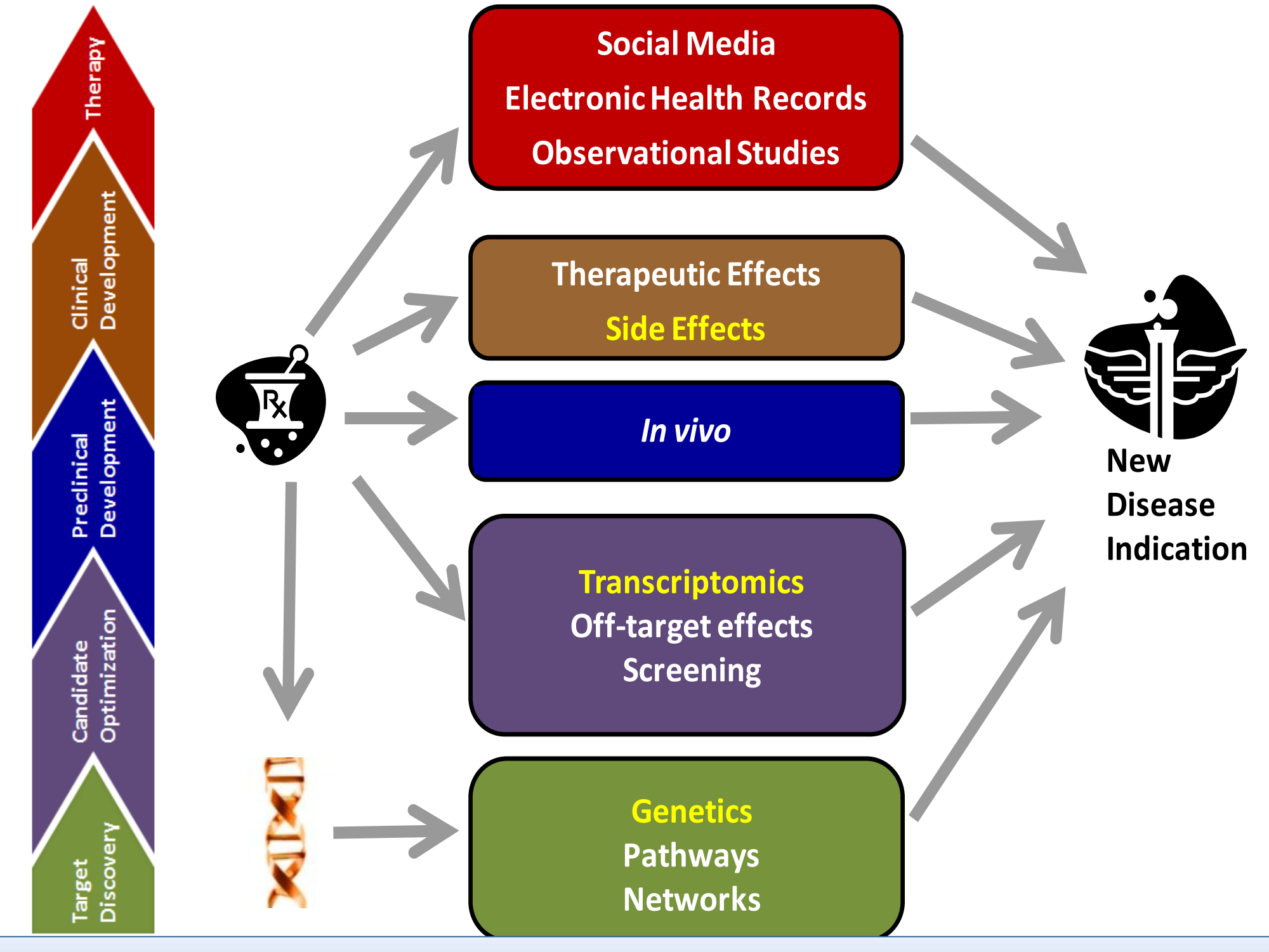
Patient Benefit: Better Safety

Corporate Benefit: Less Risk

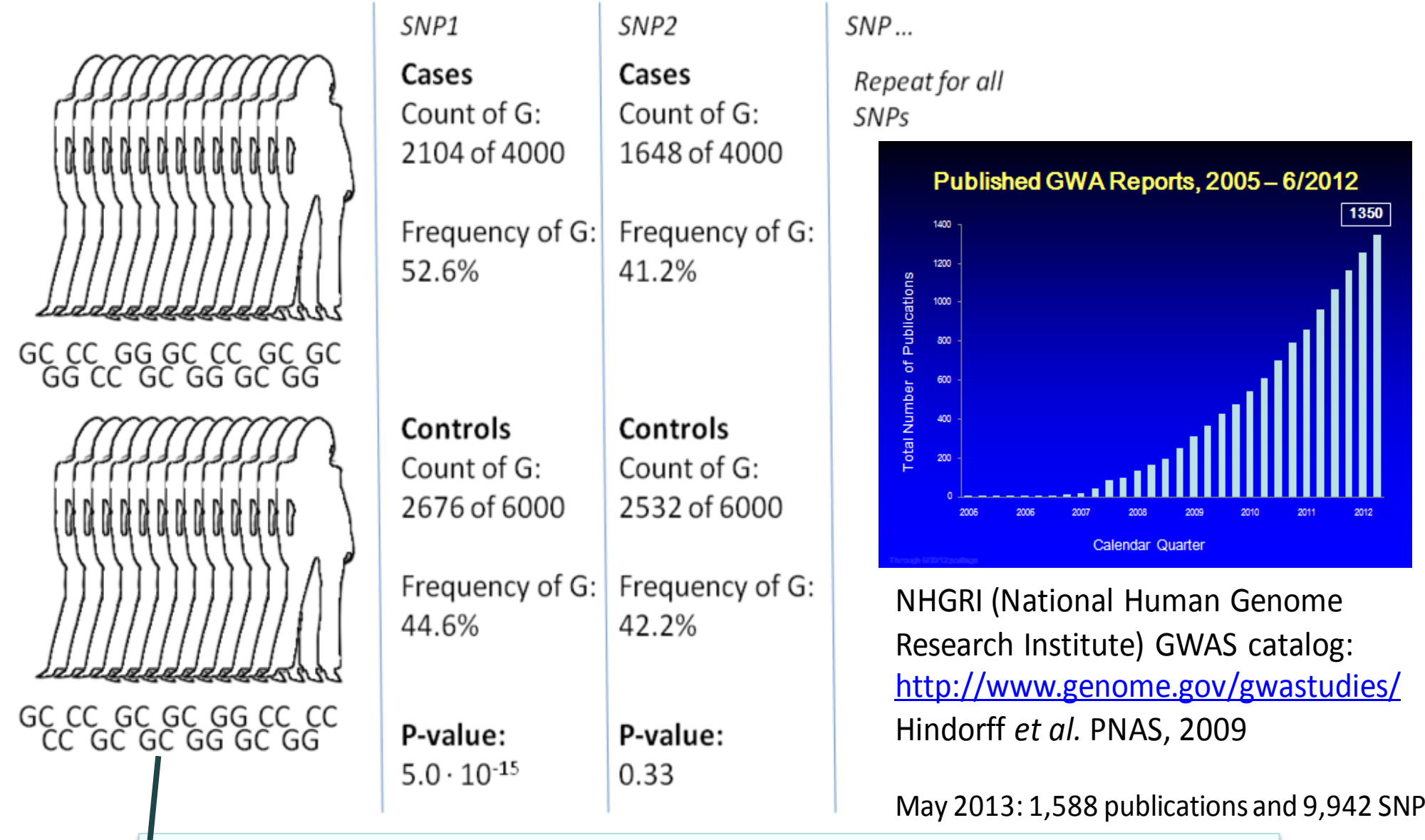
Systematic Use of Clinical Side Effects



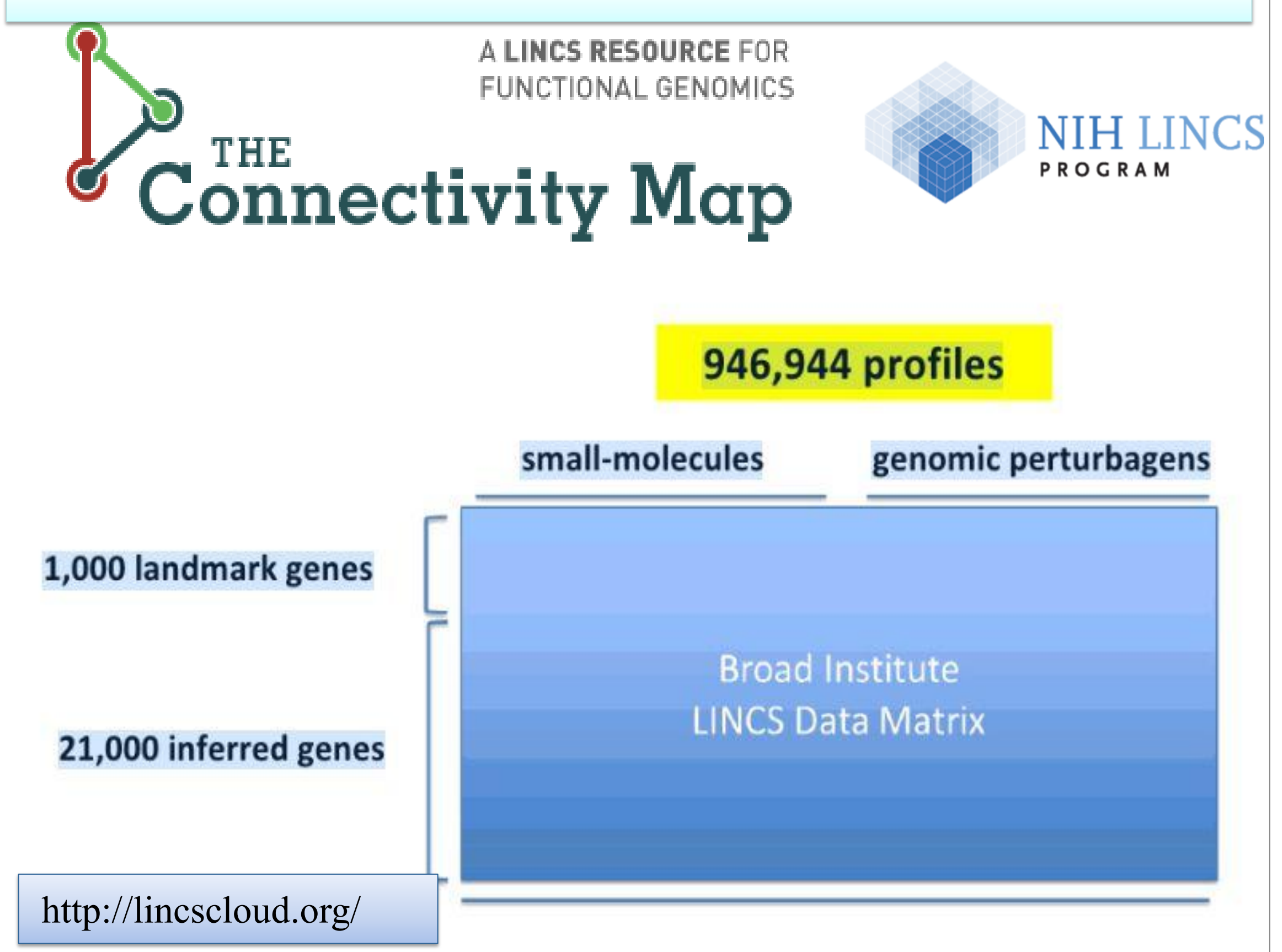
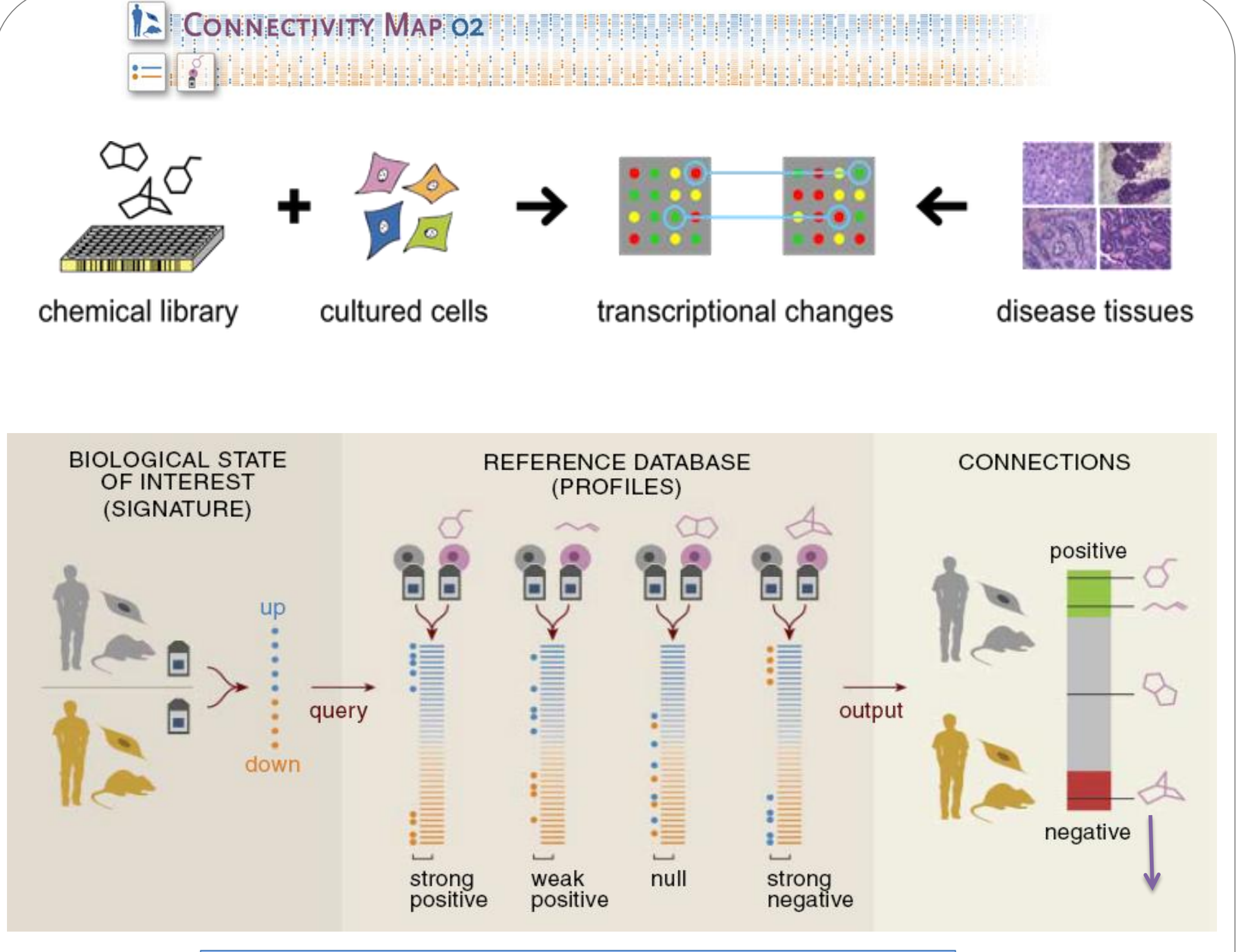
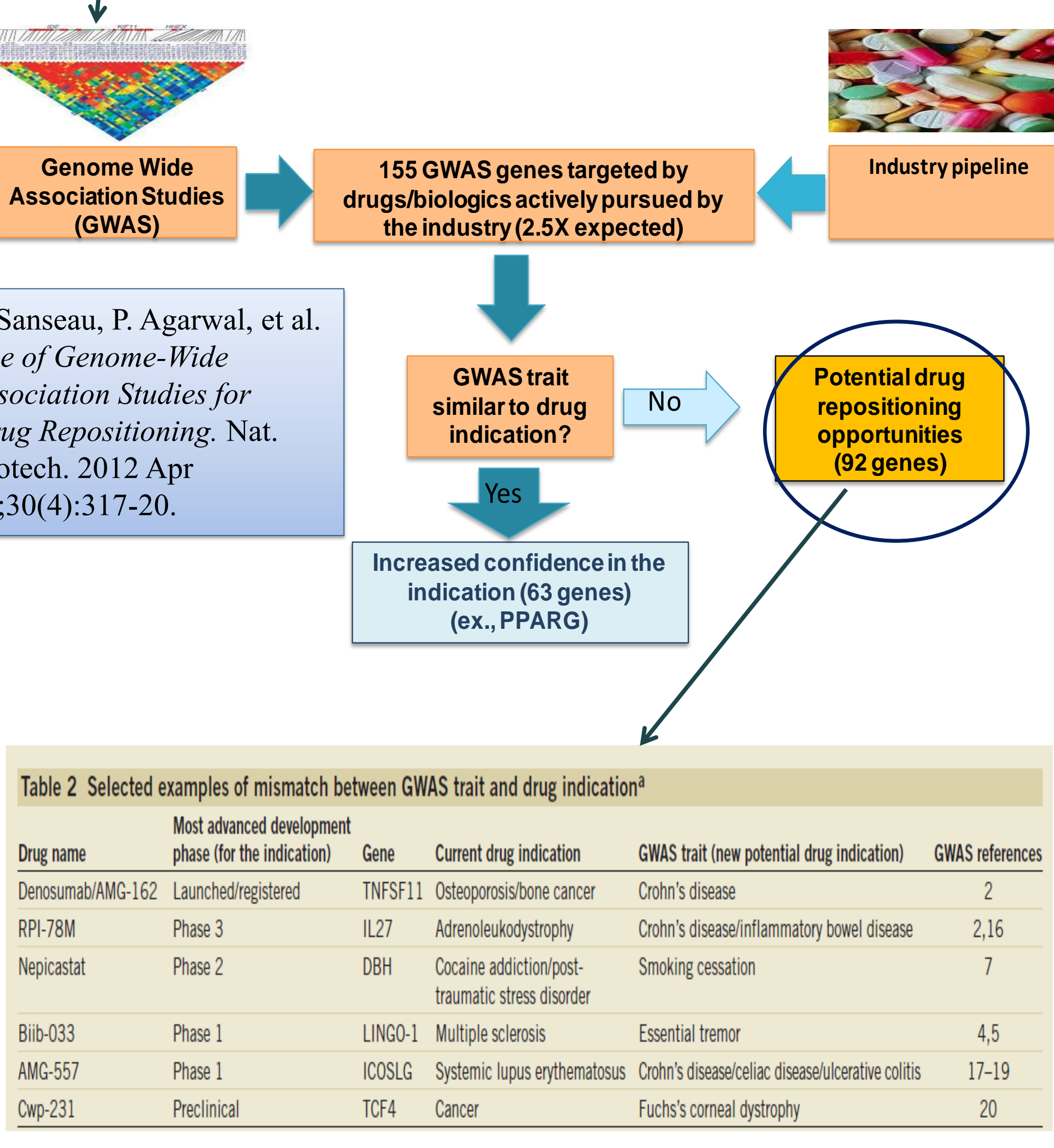
Computational Repurposing



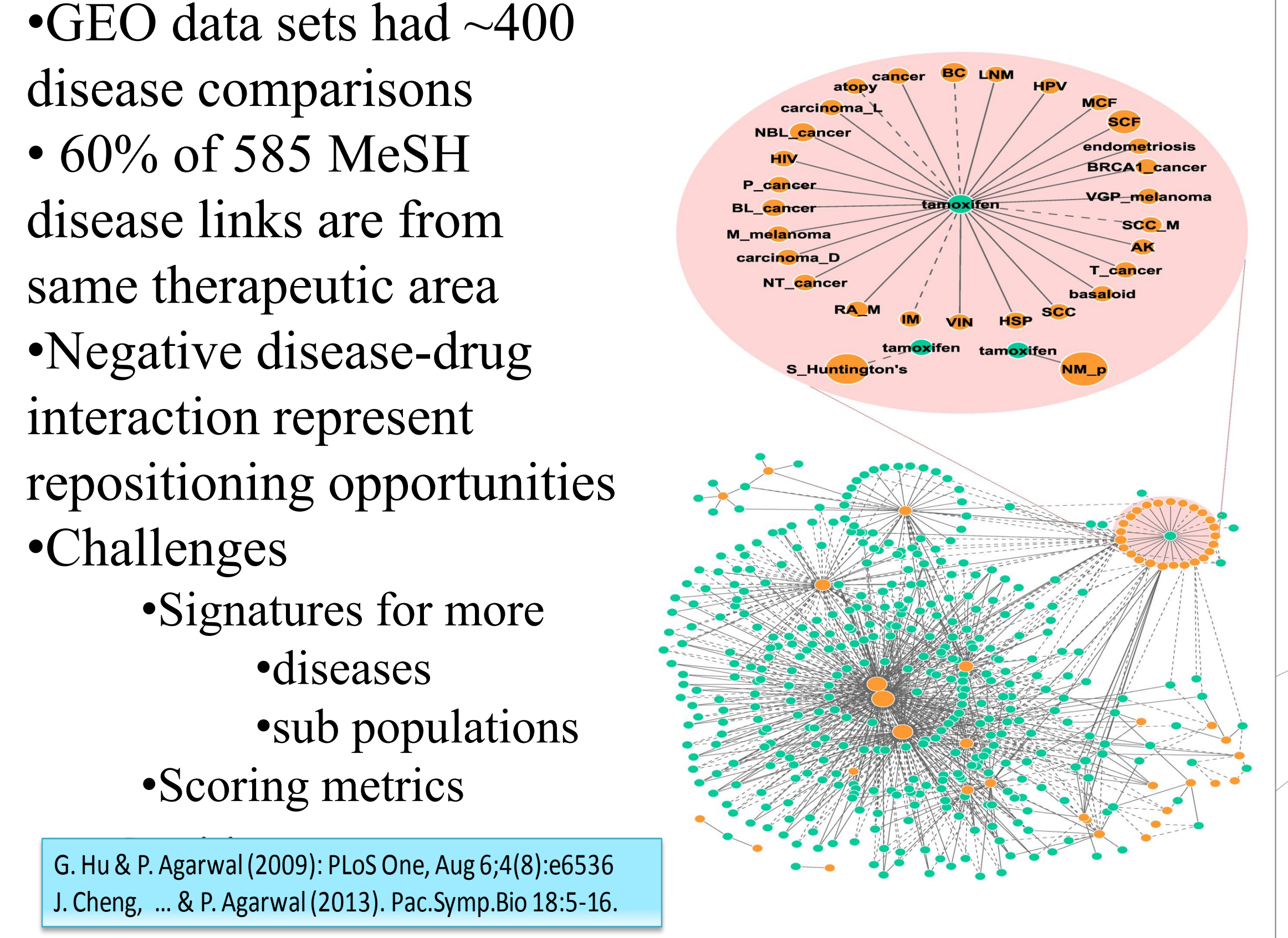
GWAS



Repurposing with GWAS



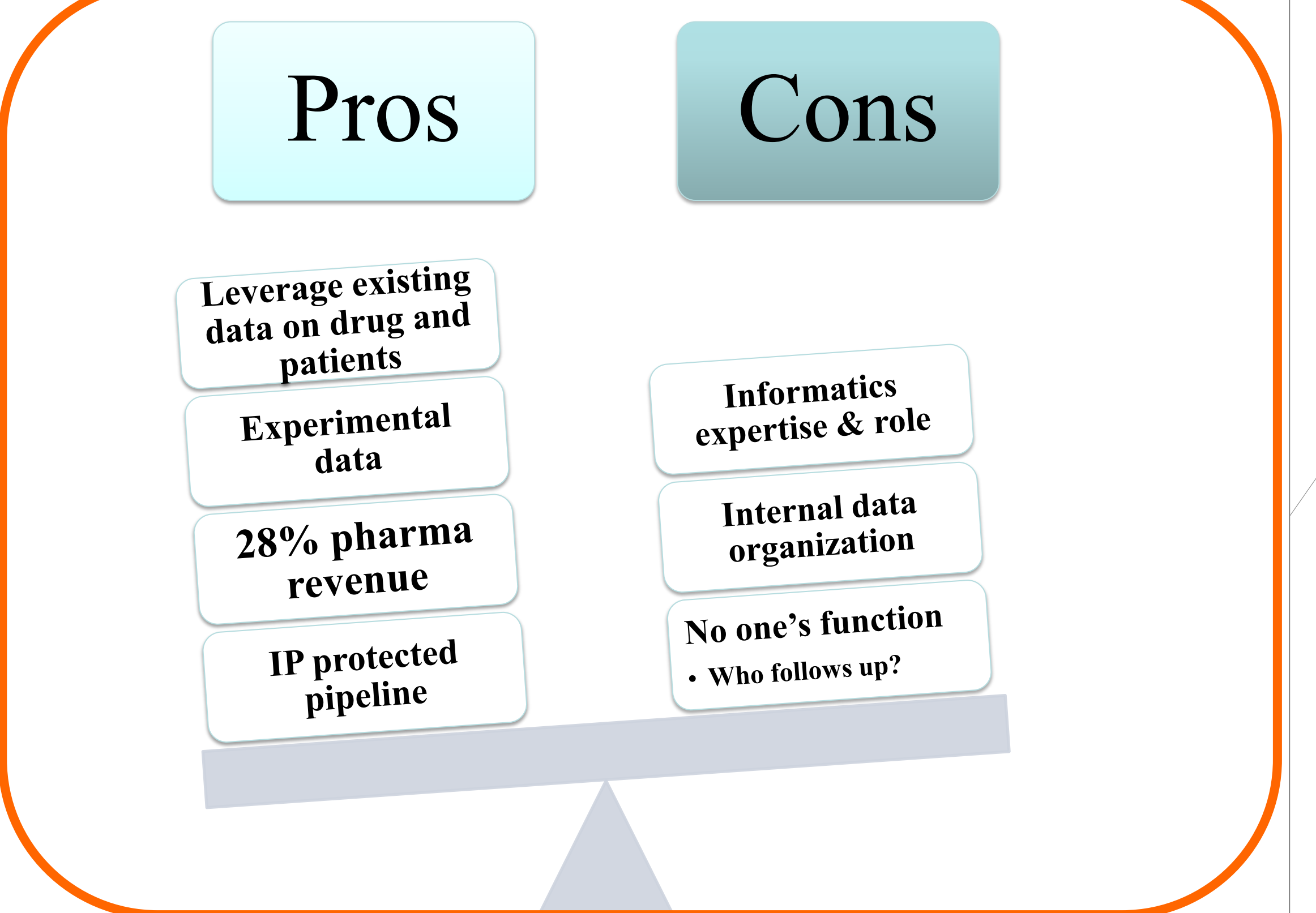
Large-scale mining



Key Evidence

- External PubMed
- P. Agarwal and D.Searls. *Can literature analysis identify innovation drivers in drug discovery?* Nat Rev Drug Discov. 2009 Nov;8(11):865-78.
- Internal Knowledge Management: Socrates Search is a Google-like application that has been enhanced for chemistry, biology and disease search. The system has indexed more than 20 terabytes of electronic lab notebooks (ELNs), Documentum archives, SharePoint sites, emails and databases. The system uses sophisticated text indexing and analytics to identify chemical structure, gene, species and disease entities. Bio-IT World 2013 Best Practices Award.

Take Home: Systematic Repurposing



M. Hurler, ..., P. Sanseau, P. Agarwal. *Computational drug repositioning: from data to therapeutics*. Clin Pharmacol Ther. 2013 Apr;93(4):335-41.

Electronic Health Records (EHRs)

