

Linking OPDDR

Open Phenotypic Drug Discovery Resource

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National Center
for Advancing
Translational Sciences



OPEN INNOVATION
DRUG DISCOVERY



DATA2DISCOVERY^{INC}



Integrative Data Science Lab
School of Informatics & Computing
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School of Medicine
University of New Mexico

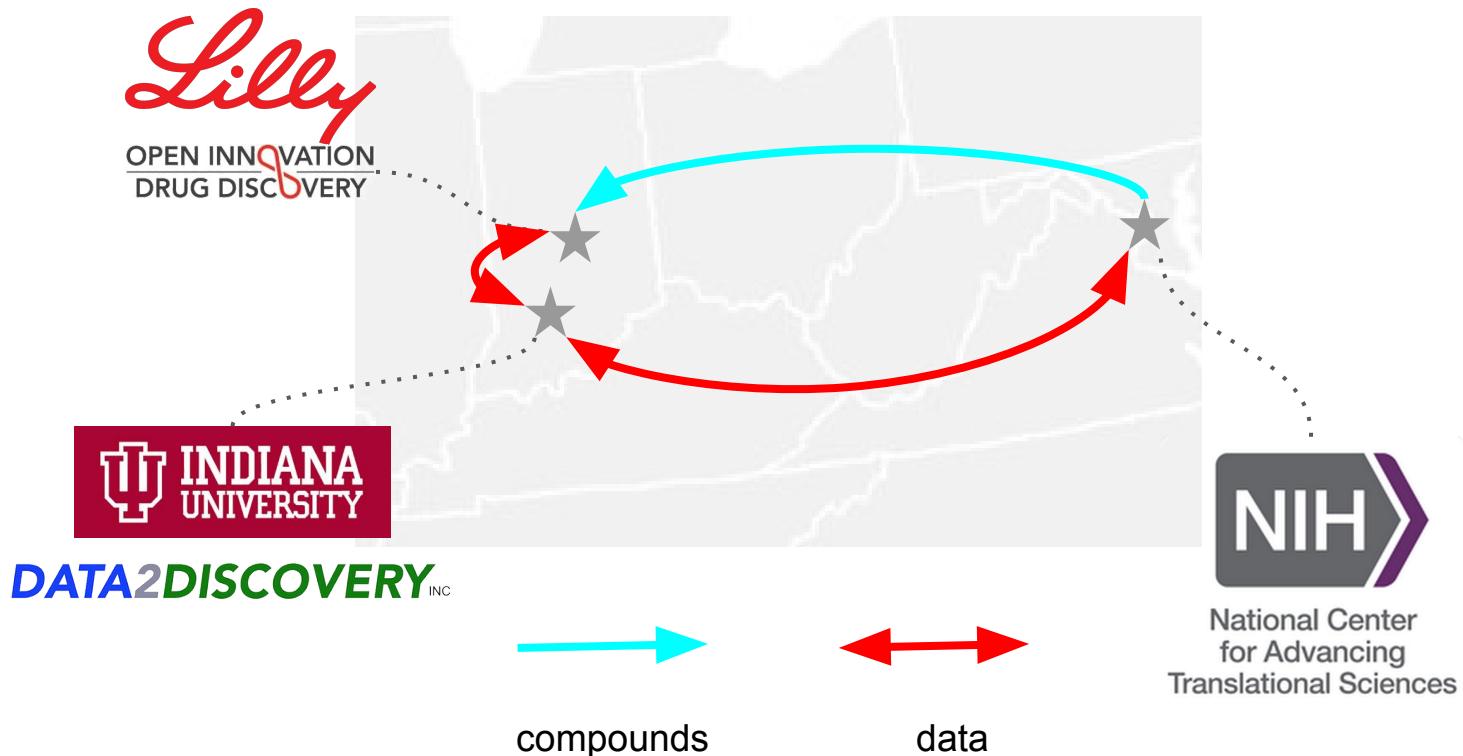
Outline

- OPDDR: project organization & overview
- Example: OIDD HeLa cell based phenotypic assay

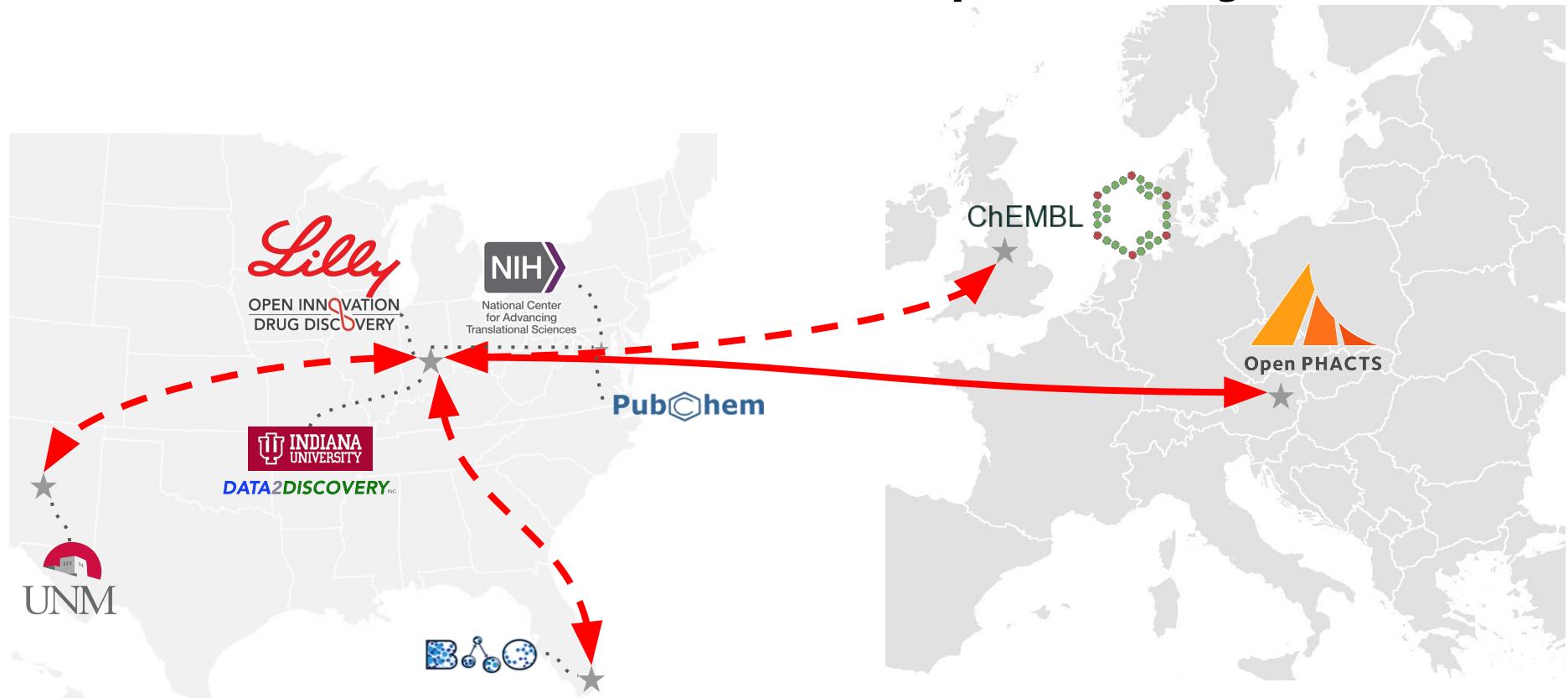
OPDDR collaboration



OPDDR collaboration



OPDDR collaboration & pathways



Example: OIDD HeLa cell based assay

- Title: “Hela CellCycMod PI MI”
- OIDD ID=17. PubChem ID=[1117350](#) (deposited 2015-03-08).
- Concentration-response assay measuring increased chromatin condensation in HeLa cells via propidium iodide staining.
- Method: cell cycle modulation
- Cell line: HeLa (human cervical adenocarcinoma)
- Fluorescence imaging
- Result type: EC50 (chromatin condensation)
- 184 tested, 31 active

Example: OIDD HeLa cell based assay

Integrated RDF

PubChem

Open

bioassay:AID1117350 rdf:type bao:BAO_0002786 .
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chembl_assay:OIDD00017 cco:hasCellLine chembl_cell_line:CHEMBL3308376 .

```
graph TD; A(( )) --> B(( )); A --> C(( )); A --> D(( ));
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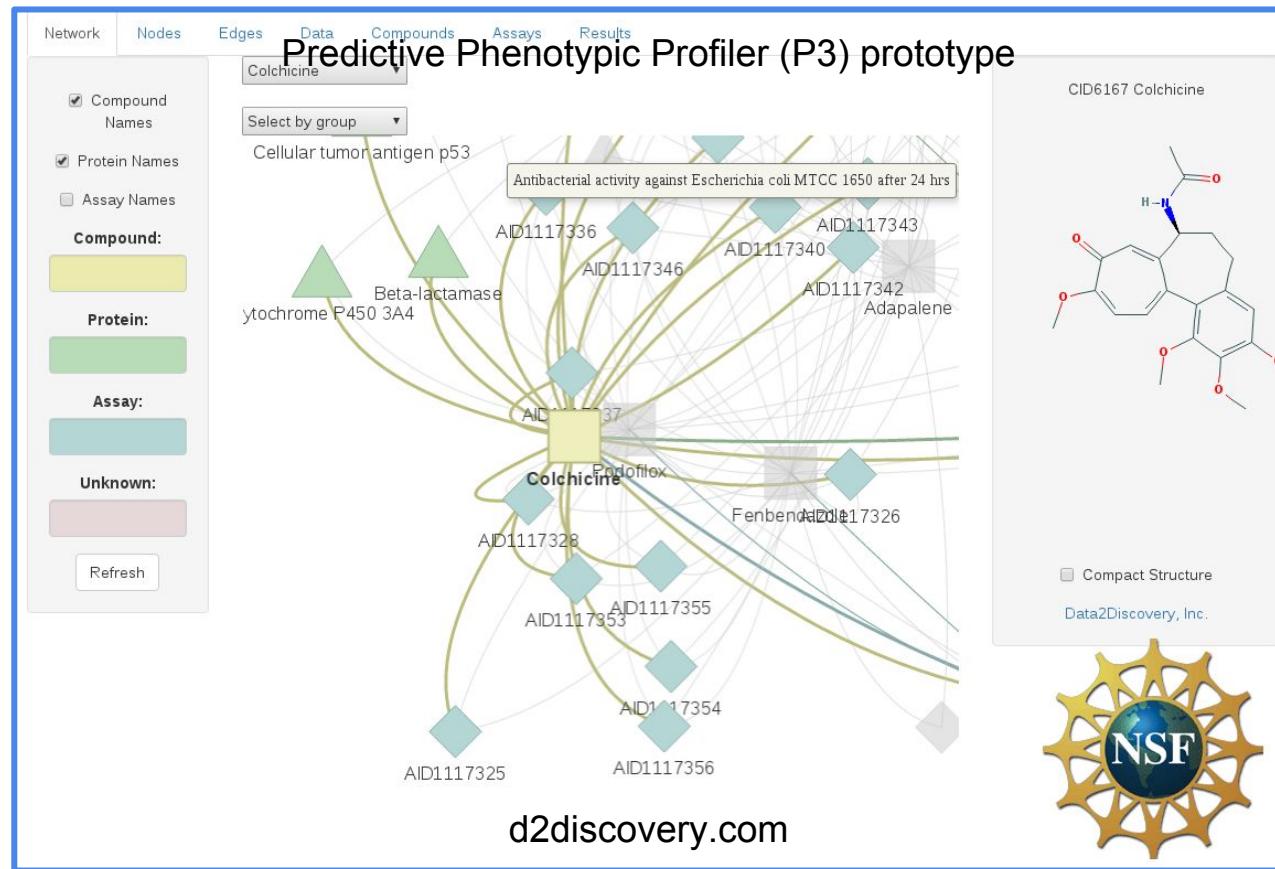
Example: OIDD HeLa cell based assay

Results, Conclusions

- OPDDR phenotypic assays have been linked and integrated via community semantics to both phenotypic (cell lines) and molecular (genomic/protein targets)
- New phenotypic knowledge domain offers additional value in drug discovery and pharmacological informatics
- Open PHACTS excellent, well suited platform

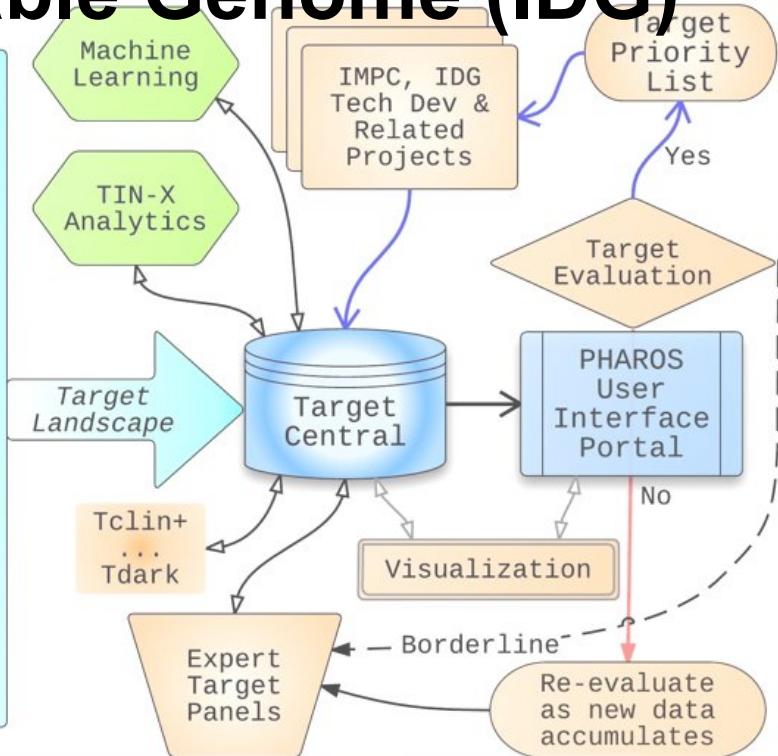
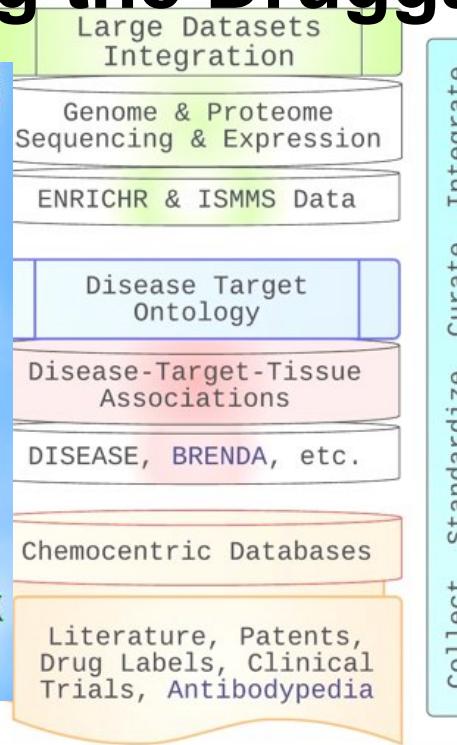
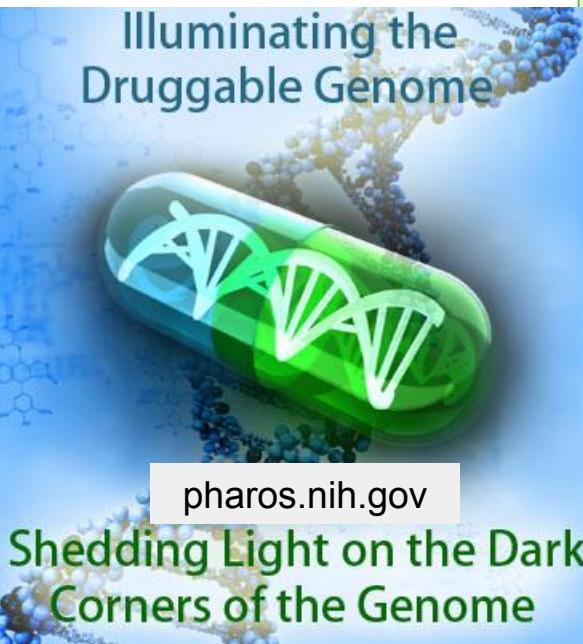
DATA2DISCOVERY INC

D2D builds apps
and solutions for
knowledge
discovery powered
by high
performance
network analytics on
rigorous semantic
standards and
platforms.



Related NIH initiative:

Illuminating the Druggable Genome (IDG)



UNM

Knowledge Mgmt Center PI:
Tudor Oprea, MD, PhD



MIAMI



Mount
Sinai



National Center
for Advancing
Translational Sciences



EMBL-EBI



The Novo Nordisk Foundation
Center for Protein Research

Acknowledgments

Lilly:

- Derek Marren
- Natalie Franklin

NCATS:

- Ajit Jadhav
- Rajarshi Guha

IU/Data2Discovery:

- David Wild
- Ying Ding

UNM:

- Tudor Oprea

Open PHACTS:

- Christine Chichester
- Nick Lynch
- Antonis Loizou
- Daniela Digles