Linking OPDDR

Open Phenotypic Drug Discovery Resource

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Outline

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

[Diagram showing collaborations between Lilly, Indiana University, DATA2DISCOVERY, and NIH, indicating exchange of compounds and data.]
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

endpoint:SID170464897_AID1117349
vocabulary:PubChemAssayOutcome vocabulary:active;
sio:has-value "0.0656"^^xsd:float;
a bao:BAO_0000190;
rdfs:label "IC50"@en .

bioassay:AID1117350 rdf:type bao:BAO_0000010 .
bioassay:AID1117350 rdf:type bao:BAO_0000219 .

substance:SID170464897
skos:exactMatch
oidd_assay:17 .

bioassay:AID1117350
skos:exactMatch
oidd_assay:17 .
bioassay:AID1117350
dcterms:source source:ID846 ;
dcterms:title "Increased chromatin condensation in HeLa cells-IC50"@en .

bioassay:AID1117350 rdf:type bao:BAO_0000010 .
bioassay:AID1117350 rdf:type bao:BAO_0000219 .

substance:SID170464897
skos:exactMatch
chembl_molecule:CHEMBL1483 .
chembl_assay:OIDD00017
cco:hasCellLine
chembl_cell_line:CHEMBL3308376 .
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
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)

Shedding Light on the Dark Corners of the Genome

Knowledge Mgmt Center PI:
Tudor Oprea, MD, PhD

pharos.nih.gov
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