Open Phenotypic Drug Discovery Resource (OPDDR)

What is the Open Phenotypic Drug Discovery Resource?

Phenotypic assays have a proven track record for generating leads that become first-in-class therapies. Whole cell assays that inform on a phenotype or mechanism also possess great potential in drug repositioning studies by illuminating new activities for the existing pharmacopeia. The National Center for Advancing Translational Sciences (NCATS) pharmaceutical collection (NPC) is the largest reported collection of approved small molecule therapeutics that is available for screening in a high-throughput setting.

Via a wide-ranging collaborative effort, this library was analyzed in the Open Innovation Drug Discovery PD2 assay modules that are publicly offered by Eli Lilly and company. The PD2 assay panel offers unique and well vetted phenotypic assessment of small molecules in five models of disease including Wnt potentiation (osteoporosis model), insulin and GLP-1 secretion (diabetes models), KRAS-Wnt synthetic lethality, and angiogenesis (cancer models).

This results obtained from the characterization of 2460 clinical phase/approved drugs in the five OIDD modules are made available on this site. A companion peer-reviewed publication describing these experiments in detail has also been submitted, and will be linked here when published.

How do I access the data?

The data is currently provided in three CSV files which contain compound metadata, assay metadata, and results. .

Compound Meta Data: NPC-OIDD-Compound.csv containing the following fields:
OIDD_SUBSTANCE: A unique substance identifier, which was assigned by Eli Lilly OIDD on receipt of the substance. There is a 1:1 mapping of OIDD_SUBSTANCE identifiers to NCGC_ID's.
NCGC_ID: A unique substance identifier assigned by NCATS; this is the same identifier used in the NPC.
PUBCHEM_SID: PubChem substance identifier
PUBCHEM_CID: PubChem parent compound identifier
SMILES: SMILES chemical structure representation, taken from PubChem
TRIVIAL NAME: Trivial name of drug

Assay Metadata: NPC-OIDD-Assay.csv containing the following fields:
OIDD_ASSAY: A unique assay identifier, assigned by Eli Lilly OIDD.
ASSAY_NAME: Name of the assay
ASSAY_METHOD: Broad category of assay type
ASSAY_TECHNOLOGY: Technology used to implement the assay
ASSAY_PROJECT: Primary therapeutic application for assay
ASSAY_SUBPROJECT: Therapeutic application sub category
ASSAY_CELL_LINE: Short identifier of cell line used
ASSAY_CELL_LINE_DESCRIPTION: Description of cell line used
ASSAY_ROLE: Screen, Primary, Secondary, Confirmatory, Profiling
RESULT_TYPE: Type of screen: IC50, EC50, %STIM, %INH
DESIRED_RESULT: Whether a positive outcome for the assay is ACTIVE or INACTIVE

SCREENING_THRESHOLD: Cutoff for determining ACTIVE/INACTIVE (NA for profiling assays)

Assay Experiment Results: NPC-OIDD-Results.csv containing the following fields:
OIDD_SUBSTANCE: Eli Lilly OIDD Unique substance identifier
OIDD_ASSAY: Lilly OIDD unique identifier for assay
CONCENTRATION: Drug concentration (for %stimulation or %inhibition assays only)
RESULT_PREFIX: Prefix for ASSAY_RESULT indicating =, < or > specified value.
ASSAY_RESULT: Assay result value (IC50, EC50, %stimulation, %inhibition)
ASSAY_OUTCOME: Assay Outcome - ACTIVE or INACTIVE
RUN_DATE: Date the assay was run

What comes next?

Eli Lilly OIDD intends to run additional screens on these compounds, and this data will be released on this site when possible. Additional semantic versions of these datasets are under development, and are expected to be released on this website soon.

How do I cite the OPDDR?

<citation will go here as “submitted” when submitted>

Contact

<Need contact at NACTS for this>

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