

Systematic annotation of bioassay protocols using ontologies

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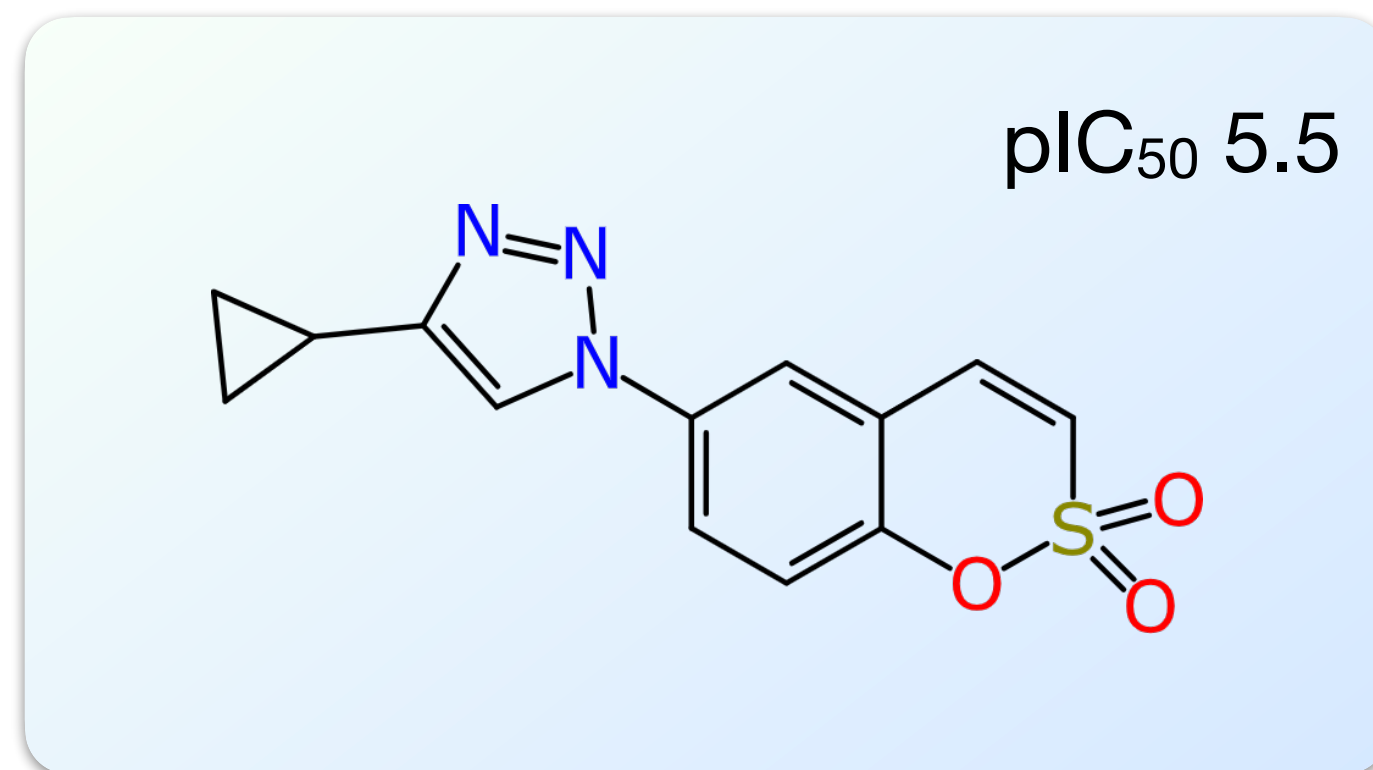
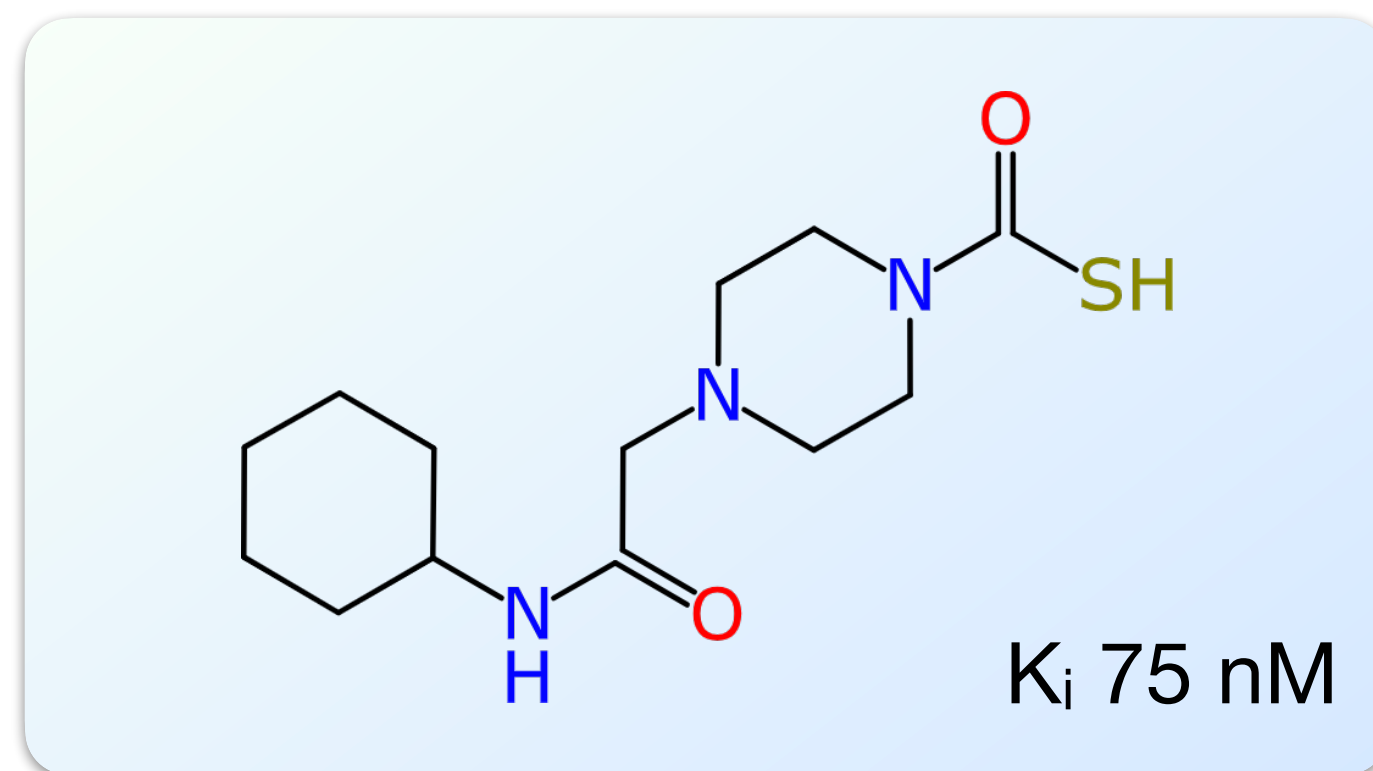
CDD VAULT[®]
Complexity Simplified



Background

- ❖ cheminformatics and bioinformatics: machine readable for decades
- ❖ ... assay informatics under-developed: measurements are rarely FAIR

machine
readable



Cell-Free Homogeneous Primary HTS to Identify Inhibitors of GSK3beta Activity

- (1) Dispense 1 μ L/well of CABPE, 0.5 μ L of ATP, and 1 μ L of positive control (GW8510 or AB) in respective wells according to plate design to 1536-well assay ready plates (Aurora 29847) that contain 2.5 nL/well of 10 mM compound using BioRAPTR (Beckman) to start the reaction. Incubate at room temperature for 60 minutes.
- (2) Add 2.5 μ L/well of ADP-glo (Promega, V9103) with BioRAPTR, incubate at room temperature for 40 minutes
- (3) Add 5 μ L/well of ADP-glo (Promega, V9103) with Combi nL (Thermo), incubate at room temperature for 30 minutes

The GSK3 β Assay Kit is designed to measure GSK3 β activity for screening and profiling applications using Kinase-Glo[®] (Promega) as a detection reagent. The GSK3 β Assay Kit comes in a convenient 96-well format, with enough purified recombinant GSK3 β enzyme, GSK3 β substrate (GSK substrate peptide), ATP, and kinase assay buffer for 100 enzyme reactions.

Assay Kit Format: Luminescent

Materials Required
Kinase-Glo[®] Max Assay (Promega #V6071)
Dithiothreitol (DTT, 1 M; optional)
Microplate reader capable of reading luminescence
Adjustable micropipettor and sterile tips
30°C incubator

not so
much...



Current best practices

- ❖ Institutions often have partially systematic assay protocol ELNs
 - ◆ e.g. *organism* or *protein target* has well defined dictionary
 - ◆ other data mostly made up of
 - **free text**
 - **pick lists**
 - **mnemonic titles**
 - **Word docs**
- ❖ Consistency between institutions is rare
- ❖ Publications usually terse, inter-referenced or implied



Ontologies to the rescue

- ❖ Public, standardized, well defined, but... how to use them?





Ontology templates

- ❖ Intermediate step:
 - ◆ select ontologies relevant to the domain
 - ◆ cherry-pick branches and place them into categories
- ❖ **Common Assay Template:** most of what you need to know for screening

bioassay type

target

detection instrument

bioassay

applies to disease

perturbagen type

format

mode of action

protein identity

design method

result

gene identity

supporting method

campaign stage

GO terms

cell line

footprint

sources

organism

assay kit

biological process

physical detection method

BioAssay templates for
the semantic web
[10.7717/peerj-cs.61](https://doi.org/10.7717/peerj-cs.61)

Template editor



Edit Ontology Template

Schema Prefix:

[Delete](#) [Download](#)

common assay template

- + bioassay type
- bioassay
 - bioassay
 - assay kit
 - experimental specification
 - bioassay specification
 - measure group
 - measure group specification
- + assay format
- + assay design method
- + assay supporting method
- + assay cell line
- + organism
- + biological process
- + target
- + applies to disease
- + assay mode of action
- + result
- + screening campaign stage
- + assay footprint
- + assay kit
- + physical detection method
- + detection instrument
- + pertubagen type
- + protein identity
- + gene identity
- + GO terms
- + assay sources
- related assays
- + **measurement**

Undo Redo

CANCEL

SAVE

Template editor



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Schema Prefix:

common assay template

- + bioassay type
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- + assay kit
- + physical detection method
- + detection instrument
- + perturbagen type
- + protein identity
- + gene identity
- + GO terms
- + assay sources
- related assays
- + measurement

Undo Redo

Edit Value

URI Custom

Look

- + absence
- assay bioassay
 - + assay kit
 - bioassay
 - + cell cycle
 - + cell growth
 - + cell morphology
 - cell motility
 - cell permeability
 - chaperone
 - + epigenetic assay
 - genotoxicity assay
 - localization assay
 - + membrane potential assay
 - + metabolomic assay
 - metastasis assay
 - organism behavior assay
 - oxidative phosphorylation assay
 - oxidative stress assay
 - + pharmacodynamic assay
 - + pharmacokinetic assay
 - + physicochemical assay
 - protein folding assay
 - protein profiling assay
 - protein stability assay
 - protein unfolding assay
 - protein-turnover assay

http://www.bioassayontology.org/bao#BAO_0000015
A set of instructions, methodology, operations, required reagents, instruments to carry out experiments for the purpose of testing the effect of a perturbing agent in a biological model system, measuring one or multiple effect(s) of the agent facilitated by an assay design method translate the perturbation into a detectable signal to arrive at one or multiple endpoint(s) that quantify or qualify the extent of the perturbation. Bioassay is described by multiple bioassay components: assay format, biology (biological participants in various role and processes), design method, physical detection method / technology, screened entity, and endpoint. Bioassay includes one or multiple measure groups to describe panel, profiling, multiparametric (or multiplexed) assays (assays that measure more than one effect of the perturbagen on the system that is screened).

Name Revert

Description Revert

Item Whole Branch Container Exclude Exclude Branch Parent URI

CANCEL

APPLY

Template editor



Edit Ontology Template

Schema Prefix:

common assay template

- + bioassay type
 - bioassay
 - bioassay
 - assay kit
 - experimental specification
 - bioassay specification
 - measure group
 - measure group specification
 - + assay format
 - + assay design method
 - + assay supporting method
 - + assay cell line
 - + organism
 - + biological process
 - + target
 - + applies to disease
 - + assay mode of action
 - + result
 - + screening campaign stage
 - + assay footprint
 - + assay kit
 - + physical detection method
 - + detection instrument
 - + perturbagen type
 - + protein identity
 - + gene identity
 - + GO terms
 - + assay sources
 - related assays
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Undo Redo

Edit Value

URI

- + absence
- assay bioassay
- + assay kit
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 - + cell cycle
 - + cell growth
 - + cell morphology
 - cell motility
 - cell permeability
 - chaperone activity
 - + epigenetic assay
 - genotoxicity assay
 - localization assay
 - + membrane potential assay
 - + metabolomic assay
 - metastasis assay
 - organism behavior assay
 - oxidative phosphorylation assay
 - oxidative stress assay
 - + pharmacodynamic assay
 - + pharmacokinetic assay
 - + physicochemical assay
 - protein folding assay
 - protein profiling assay
 - protein stability assay
 - protein unfolding assay
 - protein-turnover assay

Name

Description

Item Whole Branch Container Exclude Exclude Branch

Parent URI

CANCEL

Pick Term: bioassay

bioassay

- + cell cycle assay
- + cell growth assay
- + cell morphology assay
- cell motility assay
- cell permeability assay
- chaperone activity assay
- + epigenetic assay
- genotoxicity assay
- localization assay
- + membrane potential assay
- + metabolomic assay
- metastasis assay
- organism behavior assay
- oxidative phosphorylation assay
- oxidative stress assay
- + pharmacodynamic assay
- + pharmacokinetic assay
- + physicochemical assay
- protein folding assay
- protein profiling assay
- protein stability assay
- protein unfolding assay
- protein-turnover assay
- redistribution assay
 - dye redistribution assay
 - ion redistribution assay
 - calcium redistribution assay
 - metal ion redistribution assay
 - protein redistribution assay
 - + second messenger redistribution assay
- rna splicing assay
- + safety pharmacology assay
- sensitizer assay
- toxicity assay
- + transporter assay
- viral titer assay

Calcium functions as second messenger in cell signaling.

Search

CLOSE



Body of practice

- ❖ Use the template to create real data: set a strong precedent
- ❖ Grant funded project (*ca.* 2014):
 - ◆ create hybrid curation system: NLP & ML + expert curation
 - ◆ accelerate (rather than replace) scientists
 - ◆ gets easier and quicker as more assays are annotated
- ❖ Curated ~4000 assays from PubChem MLPCN (Molecular Libraries)
- ❖ Data can be found at:
 - ◆ <http://beta.bioassayexpress.com>
 - ◆ <https://github.com/cdd/bioassay-express>

BioAssay Express



- ❖ Built for original curation of public data
- ❖ Test-bed for many experimental features
 - ◆ data entry
 - ◆ searching
 - ◆ analysis
 - ◆ machine learning
 - ◆ text creation
 - ◆ (among others)

The screenshot displays the BioAssay Express web interface for editing an assay. The browser address bar shows the URL: `beta.bioassayexpress.com/assign.jsp?assayID=7008&edit=true`. The page title is "BioHarmony: Annotator" with the tagline "Metadata Simplified". The main heading is "Assign Assay".

At the top right, there are buttons for "Submit", "New", and "Clone", along with a search box labeled "find by ID" and a "Login" button. Below this is a search bar "find term to annotate with".

The interface is divided into several sections:

- PubChem Assay ID:** 743348
- Origin:** common assay template
- Template:** Sections, Undo, Redo

The main content area is split into three vertical panels:

- Protocol Text:** Contains the assay title "HepG2 Cytotoxicity Assay Measured in Cell-Based System Using Plate Reader - 7071-02_Inhibitor_Dose_DryPowder_Activity_Set10" and keywords: "Cytotoxicity Assay, luminescence, CellTiter-Glo, HepG2".
- Assay Annotations:** A list of fields with dropdown menus and tags. Fields include: assay title, bioassay type (functional), bioassay (cell viability ATP quantitation assay), assay format (cell based format), assay design method (ATP quantitation using luciferase), assay supporting method, assay cell line (Hep-G2 cell), organism (Homo sapiens), biological process (cell population proliferation), target (n/a), applies to disease (n/a), assay mode of action (growth inhibition), result (AC50), screening campaign stage (compound toxicity assay), assay footprint (384 well plate), assay kit (CellTiter-Glo Luminescent Cell Viability Assay), physical detection method (bioluminescence), detection instrument (EnVision Multilabel Reader), perturbagen type (unknown), protein identity, gene identity, GO terms, assay sources (Broad Institute (Harvard-MIT)), related assays (AID 623896), measurement (AC50_uM), and units (micromolar).
- Similar Assays:** A list of similar assay IDs: AID 651898, AID 652117, AID 652118, AID 720585, AID 720594, AID 743185, AID 743354, AID 743358, AID 624285, AID 651860. A search box is at the bottom.

At the bottom of the Protocol Text panel, there is an "Autogenerated Text" section with two paragraphs of text summarizing the assay details.



What can you do with marked up assays?

- ❖ Search by narrowing with *exact* and *precise* criteria

The screenshot shows a search interface with a dropdown menu for 'LAYER 1' and a search bar containing 'bioassay type'. Below the search bar, a list of assay types is displayed, each with a radio button and a count in parentheses. The 'binding type' option is highlighted with a black background. The list includes:

- empty ?
- with text ?
- bioassay type ? (with thumbs up and thumbs down icons)
 - ADMET ? (554) (with thumbs up and thumbs down icons)
 - Toxicity ? (124)
 - **binding type** ? (1105)
 - + functional ? (4321) (with thumbs up and thumbs down icons)
 - physicochemical ? (66)
 - + absence ? (with thumbs up and thumbs down icons)

- ❖ Can also use annotations like fingerprints



What can you do with marked up assays?

- ❖ Search by narrowing with *exact* and *precise* criteria

▼ LAYER 1 bioassay type Keywords:

- empty ?
- with text ?
- bioassay type ? | |
- ADMET ? (554) | |
- Toxicity ? (124)
- **binding type** ? (1105)
- + functional ? (4321) | |
- physicochemical ? (66)
- + absence ? | |

▼ LAYER 2 organism Keywords:

- empty ?
- with text ?
- organism ? | |
- cellular organisms ? | |
- eukaryote ? | |
- fungi ? | |
- unicellular fungi ? | |
- Saccharomyces cerevisiae ? (1 of 98)
- metazoa ? | |
- invertebrate ? | |
- Caenorhabditis elegans ? (9 of 25)
- Photinus pyralis ? (1 of 19)
- vertebrate ? | |
- mammalian ? | |
- Bos taurus ? (6 of 13)
- Canis lupus familiaris ? (3 of 52)
- Cavia porcellus ? (8 of 11)
- Homo sapiens ? (971 of 4141)
- **Mus musculus** ? (44 of 367)
- + Primates ? | |
- **Rattus norvegicus** ? (15 of 335)
- protozoan ? | |
- Plasmodium falciparum ? (1 of 47)
- Plasmodium falciparum 3D7 ? (2 of 3)
- + prokaryote ? | |
- + virus ? | |
- + absence ? | |

- ❖ Can also use annotations like fingerprints



What can you do with marked up assays?

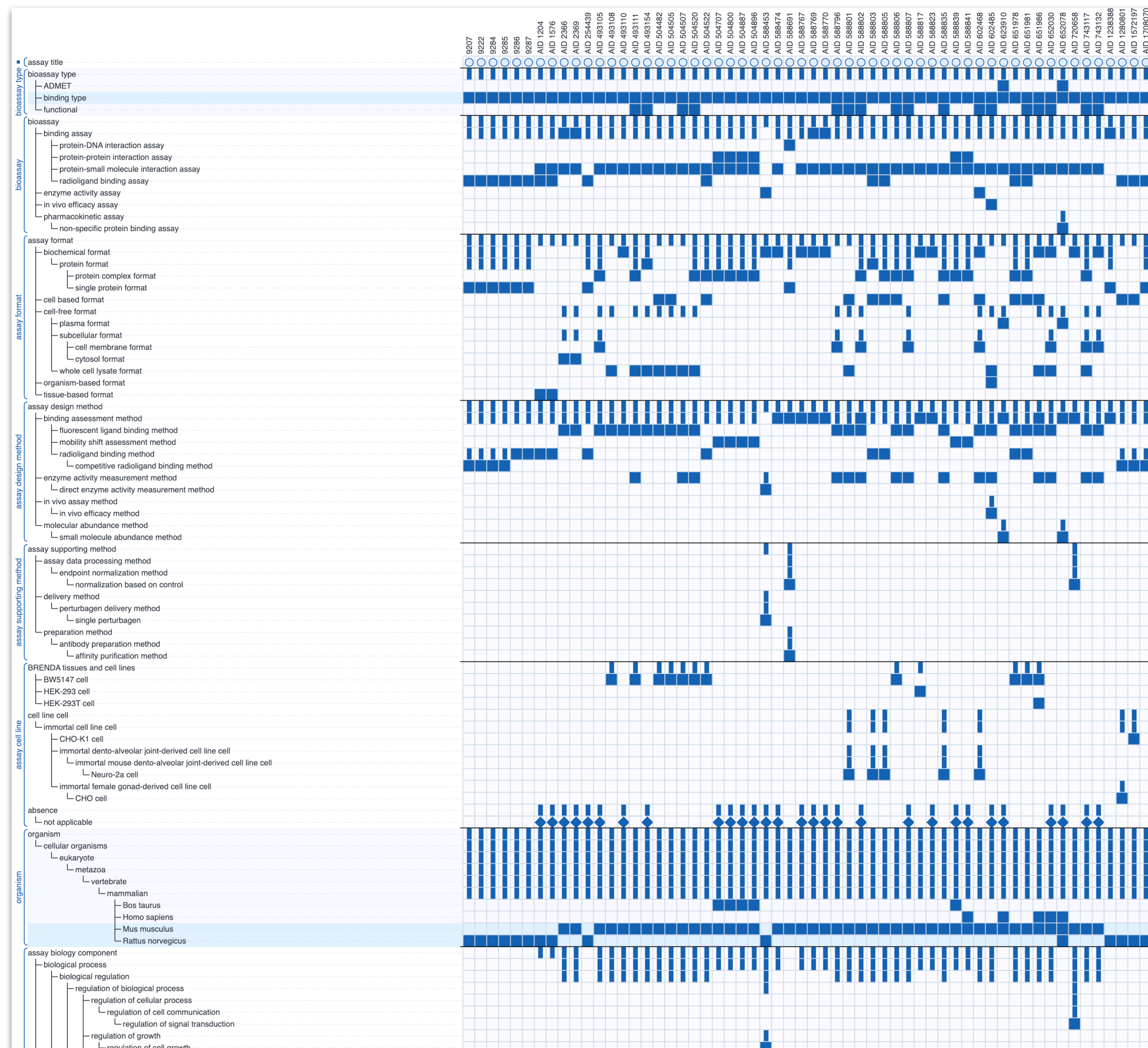
❖ Search by narrowing with *exact* and *precise* criteria

▼ LAYER 1 bioassay type Keywords:

- empty ?
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▼ LAYER 2 organism Keywords:

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 - Saccharomyces cerevisiae ? (1 of 98)
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- + virus ?
- + absence ?



❖ Can also use annotations like fingerprints



What can you do with marked up assays?

❖ Search by narrowing with *exact* and *precise* criteria

The screenshot displays a search interface for bioassays with the following components:

- LAYER 1: bioassay type**
 - Keywords:
 - empty ?
 - with text ?
- LAYER 2: organism**
 - Keywords:
 - empty ?
 - with text ?
 - organism ?
 - cellular organisms ?
- assay format**
 - biochemical format
 - protein format
 - protein complex format
 - single protein format
 - cell based format
 - cell-free format
 - plasma format
 - subcellular format
 - cell membrane format
 - cytosol format
 - whole cell lysate format
 - organism-based format
 - tissue-based format
- organism**
 - protozoan ?
 - Plasmodium falciparum ? (1 of 47)
 - Plasmodium falciparum 3D7 ? (2 of 3)
 - prokaryote ?
 - virus ?
 - absence ?
- assay biology component**
 - biological regulation
 - regulation of biological process
 - regulation of cellular process
 - regulation of cell communication
 - regulation of signal transduction
 - regulation of growth
 - regulation of cell growth

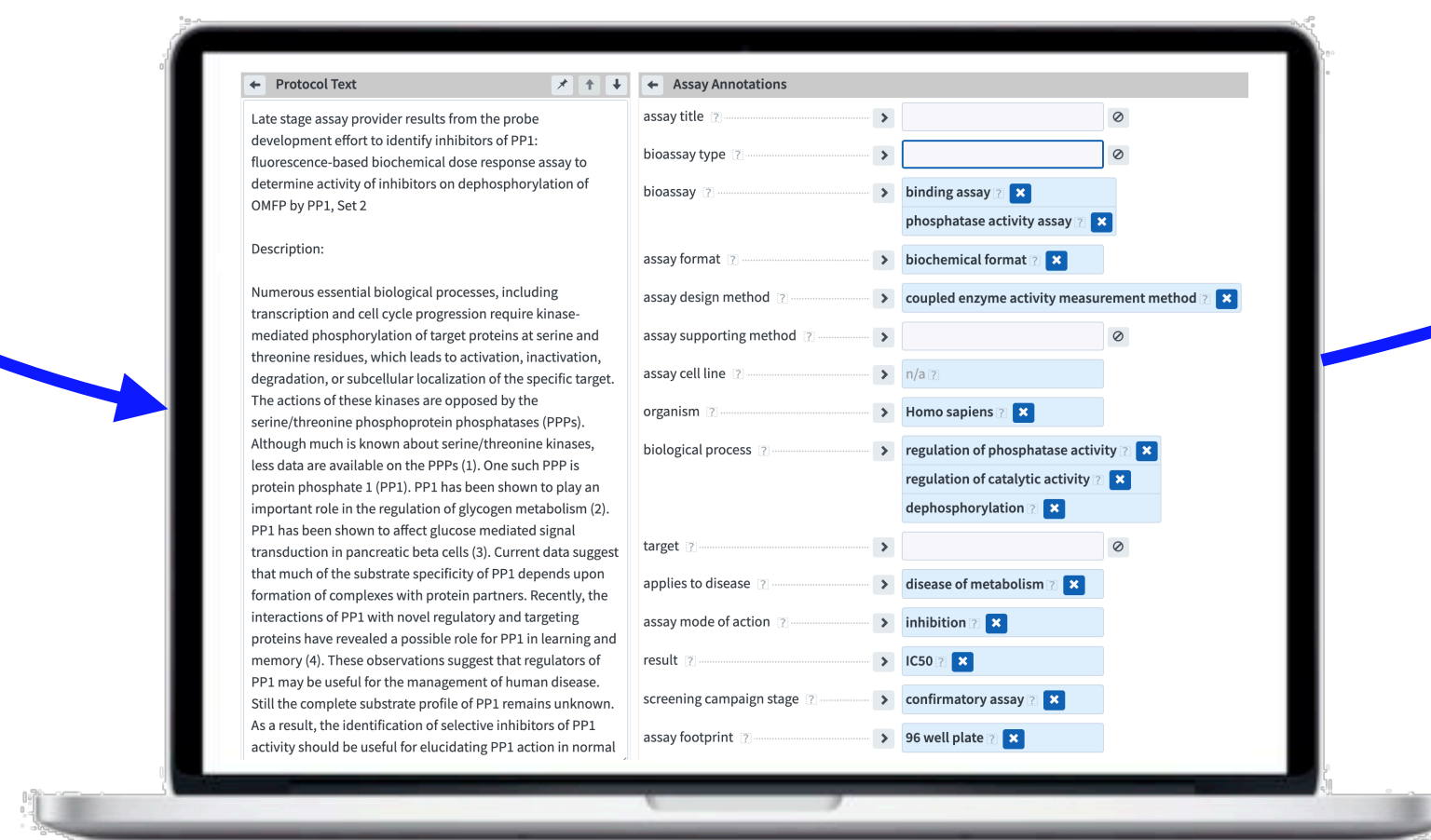
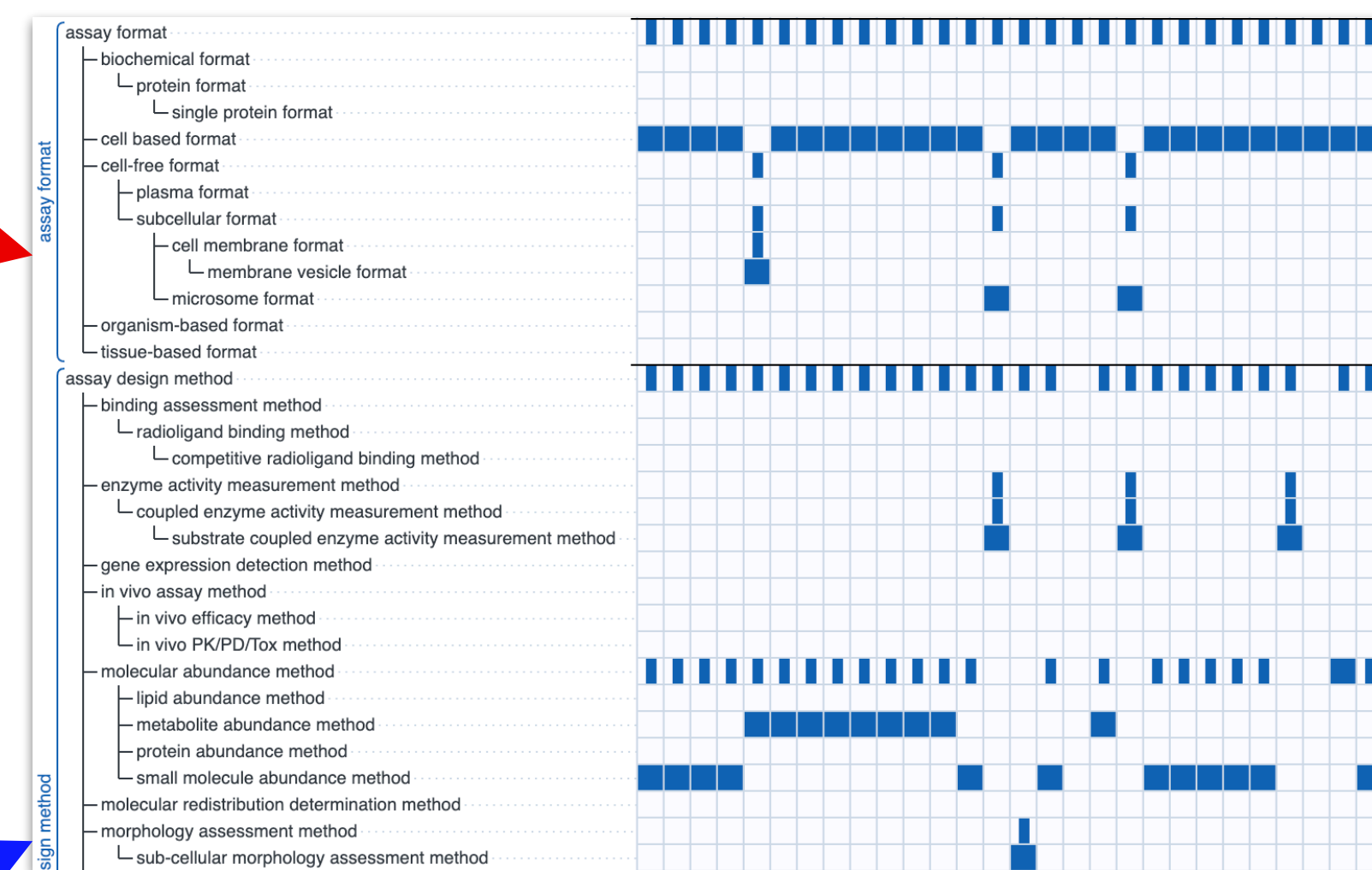
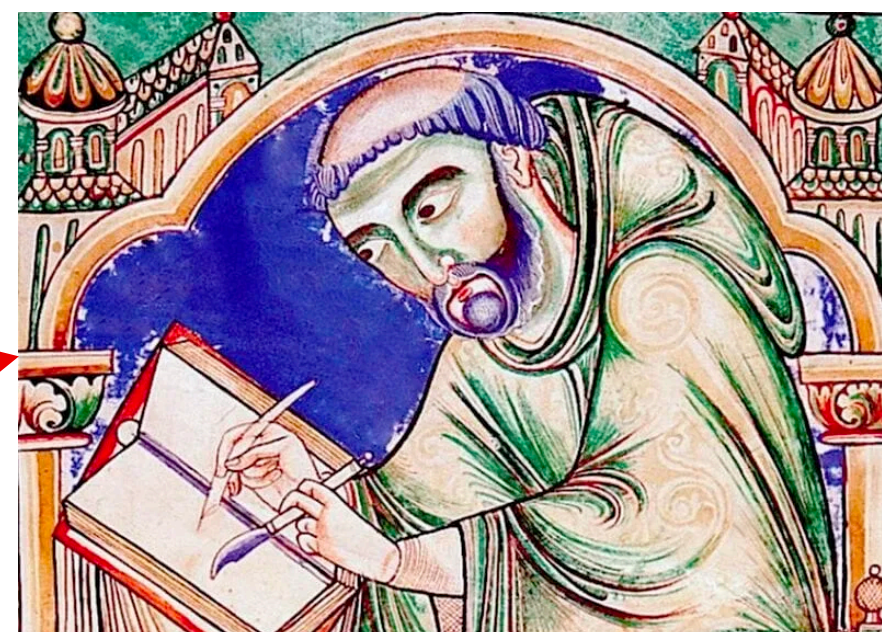
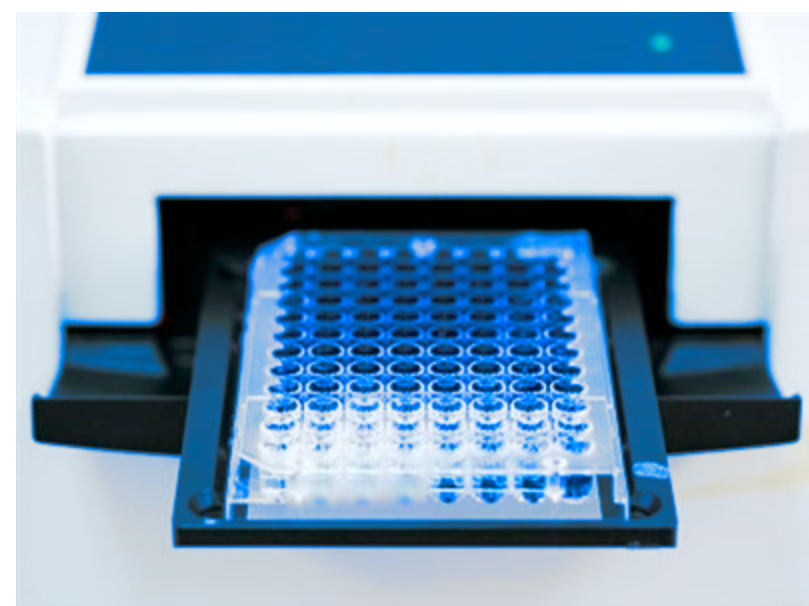
The main area of the interface is a heatmap where rows represent the categories above and columns represent individual assays (e.g., AID 9207, AID 9222, AID 9284, AID 9285, AID 9286, AID 9287, AID 1204, AID 1576, AID 2366, AID 2369, AID 254439, AID 493105, AID 493108, AID 493110, AID 493111, AID 493154, AID 504482, AID 504505, AID 504507, AID 504522, AID 504522, AID 504707, AID 504900, AID 504987, AID 504986, AID 588453, AID 588474, AID 588891, AID 588891, AID 588769, AID 588770, AID 588796, AID 588801, AID 588802, AID 588803, AID 588805, AID 588806, AID 588807, AID 588817, AID 588823, AID 588835, AID 588839, AID 588841, AID 602468, AID 602468, AID 602468, AID 651976, AID 651981, AID 651986, AID 652030, AID 652078, AID 720658, AID 743117, AID 743132, AID 1238388, AID 1280801, AID 1572197, AID 1708070).

❖ Can also use annotations like fingerprints



Curation: now vs. then

❖ Writing up text, then re-deriving machine readable description... ?



❖ Make the FAIR UI *easier*

❖ Introduce short term payoffs



Annotation as a product

- ❖ **BioAssay Express**: advanced prototype, open source
- ❖ **CDD Vault Annotations**: 80/20 rule, same data model
- ❖ Vault is used daily by thousands of scientists, meet them where they're at
- ❖ Knowing about the *semantic web* is optional
- ❖ Introduce ontologies and templates gently
 - ◆ well defined set of terms
 - ◆ everyone has access to same vocabulary
 - ◆ like what they had before, except better

The screenshot displays the CDD Vault Probes Vault interface. The top navigation bar includes 'CDD.VAULT · Probes Vault', 'Help', and 'Log out'. Below this is a secondary navigation bar with 'Explore Data', 'Import Data', 'Reports', 'Settings', and a user profile 'Alex Clark'. The main content area features a search bar, a list of projects (e.g., 'Projects', 'ADMEdata.com for Ekins Ca...', 'Alex Clark Sandbox'), and a list of molecules. The molecule list shows 2815 molecules, with the first few entries including chemical structures, names (e.g., JHU-12792, CDD-2655024), and associated data (Synonyms: (no synonyms), Protocols: 5). The URL at the bottom of the browser window is <https://app.collaborativedrug.com/vaults/4126/molecules/4758311>.



Protocol forms

- ❖ Mix text, numbers & pick lists with selected ontology terms

Edit Form: In-vitro Mouse Cancer Screening

Protocol Definition Run Definition

Form Name*
In-vitro Mouse Cancer Screening

Protocol Name *

Category *

Description

Instrument

bioassay type **assay format**

organism

applies to disease

physical detection method

Text

Protocol Fields ?

Category

Description

Instrument

common assay template

bioassay type

bioassay

assay format

assay design method

assay supporting method

assay cell line

organism

biological process

Delete Cancel **Save**



Protocol forms

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Protocol Definition | Run Definition

Form Name*
In-vitro Mouse Cancer Screening

Protocol Name *

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Instrument

bioassay type Annotation Free Text

assay format Annotation Free Text

organism Annotation Free Text

applies to disease Annotation Free Text

physical detection method Annotation Free Text

Text

Protocol Fields ?

Category

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common assay template

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bioassay

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biological process

Delete Cancel

Run Data | **Protocol Details** | Projects 1 | Files 0

Form

Protocol Name * Special characters

Category *

Description

Instrument

bioassay type Annotation Free Text **assay format** Annotation Free Text

organism Annotation Free Text

applies to disease Annotation Free Text

physical detection method Annotation Free Text

CANCEL



Business logic

- ❖ Reduce curation efforts
- ❖ *and* fewer mistakes

bioassay type ⊕ Annotation ⊕ Free Text ✎	assay format ⊕ Annotation ⊕ Free Text ✎
organism ⊕ Annotation ⊕ Free Text ✎	
applies to disease ⊕ Annotation ⊕ Free Text ✎	
physical detection method ⊕ Annotation ⊕ Free Text ✎	



Business logic

- ❖ Reduce curation efforts
- ❖ *and* fewer mistakes

default

Pick Term: bioassay type

- bioassay type
 - ADMET
 - binding type
 - **functional**
 - functional phenotypic
 - functional target-based
 - physicochemical

bioassay type	⊕ Annotation	⊕ Free Text	✎	assay format	⊕ Annotation	⊕ Free Text	✎
organism	⊕ Annotation ⊕ Free Text ✎						
applies to disease	⊕ Annotation ⊕ Free Text ✎						
physical detection method	⊕ Annotation ⊕ Free Text ✎						



Business logic

- ❖ Reduce curation efforts
- ❖ *and* fewer mistakes

Pick Term: organism

organism

- cellular organisms
- eukaryote
- + fungi
- metazoa
- + invertebrate
- vertebrate
- mammalian
 - Bos taurus
 - Canis lupus familiaris
 - Capra hircus
 - Cavia porcellus
 - Cercopithecidae
 - Cervus canadensis nelsoni
 - Chinchilla lanigera
 - Chlorocebus aethiops
 - Chlorocebus aethiops
 - Cricetinae
 - Equus caballus
 - Felis catus
 - Homo sapiens
 - marmosets
 - Marmota monax
 - Mastomys coucha
 - Meriones unguiculatus
 - Mesocricetus auratus
 - Microtus ochrogaster
 - Murinae
 - **Mus musculus**
 - Mustela putorius furo
 - Oryctolagus cuniculus
 - Ovis aries
 - Pan troglodytes
 - Papio anubis
 - Papio hamadryas
 - Potorous tridactylus

default

Pick Term: bioassay type

bioassay type

- ADMET
- binding type
- **functional**
- functional phenotypic
- functional target-based
- physicochemical

locked

bioassay type ⊕ Annotation ⊕ Free Text ✎

assay format ⊕ Annotation ⊕ Free Text ✎

organism ⊕ Annotation ⊕ Free Text ✎

applies to disease ⊕ Annotation ⊕ Free Text ✎

physical detection method ⊕ Annotation ⊕ Free Text ✎



Business logic

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Pick Term: organism

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Pick Term: bioassay type

bioassay type

- ADMET
- binding type
- **functional**
- functional phenotypic
- functional target-based
- physicochemical

Pick Term: applies to disease

Disease

- + disease by infectious agent
- + disease of anatomical entity
- disease of cellular proliferation
- + benign neoplasm
- cancer
 - + cell type cancer
 - head and neck cancer
 - organ system cancer
 - + cardiovascular cancer
 - endocrine gland cancer
 - + neuroendocrine tumor
 - **pancreatic cancer**
 - islet cell tumor
 - insulinoma
 - pancreatic endocrine carcinoma
 - pancreatic gastrinoma
 - pancreatic somatostatinoma
 - malignant exocrine pancreas neoplasm
 - pancreatic carcinoma
 - pancreatic ductal carcinoma
 - pancreatoblastoma
 - + pineal gland cancer
 - + pituitary cancer
 - + thymus cancer
 - + peritoneum cancer
 - + reproductive organ cancer
 - + retroperitoneal cancer
 - + thoracic cancer
 - + urinary system cancer
 - + pre-malignant neoplasm
- + disease of mental health
- + disease of metabolism
- + genetic disease
- + physical disorder
- + syndrome

default

subset

locked

bioassay type ⊕ Annotation ⊕ Free Text ✎ assay format ⊕ Annotation ⊕ Free Text ✎

organism ⊕ Annotation ⊕ Free Text ✎

applies to disease ⊕ Annotation ⊕ Free Text ✎

physical detection method ⊕ Annotation ⊕ Free Text ✎

Business logic

- ❖ Reduce curation efforts
- ❖ *and* fewer mistakes



Pick Term: organism

organism

- cellular organisms
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 - Bos taurus
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 - Chlorocebus aethiops
 - Cricetinae
 - Equus caballus
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 - Papio anubis
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Pick Term: bioassay type

bioassay type

- ADMET
- binding type
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- functional phenotypic
- functional target-based
- physicochemical

Pick Term: applies to disease

Disease

- + disease by infectious agent
- + disease of anatomical entity
- disease of cellular proliferation
- + benign neoplasm
- cancer
 - + cell type cancer
 - head and neck cancer
 - organ system cancer
 - + cardiovascular cancer
 - endocrine gland cancer
 - + neuroendocrine tumor
 - **pancreatic cancer**
 - islet cell tumor
 - insulinoma
 - pancreatic endocrine carcinoma
 - pancreatic gastrinoma
 - pancreatic somatostatinoma
 - malignant exocrine pancreas neoplasm
 - pancreatic carcinoma
 - pancreatic ductal carcinoma
 - pancreatoblastoma
 - + pineal gland cancer
 - + pituitary cancer
 - + thymus cancer
- + peritoneum cancer
- + reproductive organ cancer
- + retroperitoneal cancer
- + thoracic cancer
- + urinary system cancer

- + pre-malignant neoplasm
- + disease of mental health
- + disease of metabolism
- + genetic disease
- + physical disorder
- + syndrome

bioassay type ⊕ Annotation ⊕ Free Text ✎ assay format ⊕ Annotation ⊕ Free Text ✎

organism ⊕ Annotation ⊕ Free Text ✎

applies to disease ⊕ Annotation ⊕ Free Text ✎

physical detection method ⊕ Annotation ⊕ Free Text ✎

Pick Term: physical detection method

physical detection method

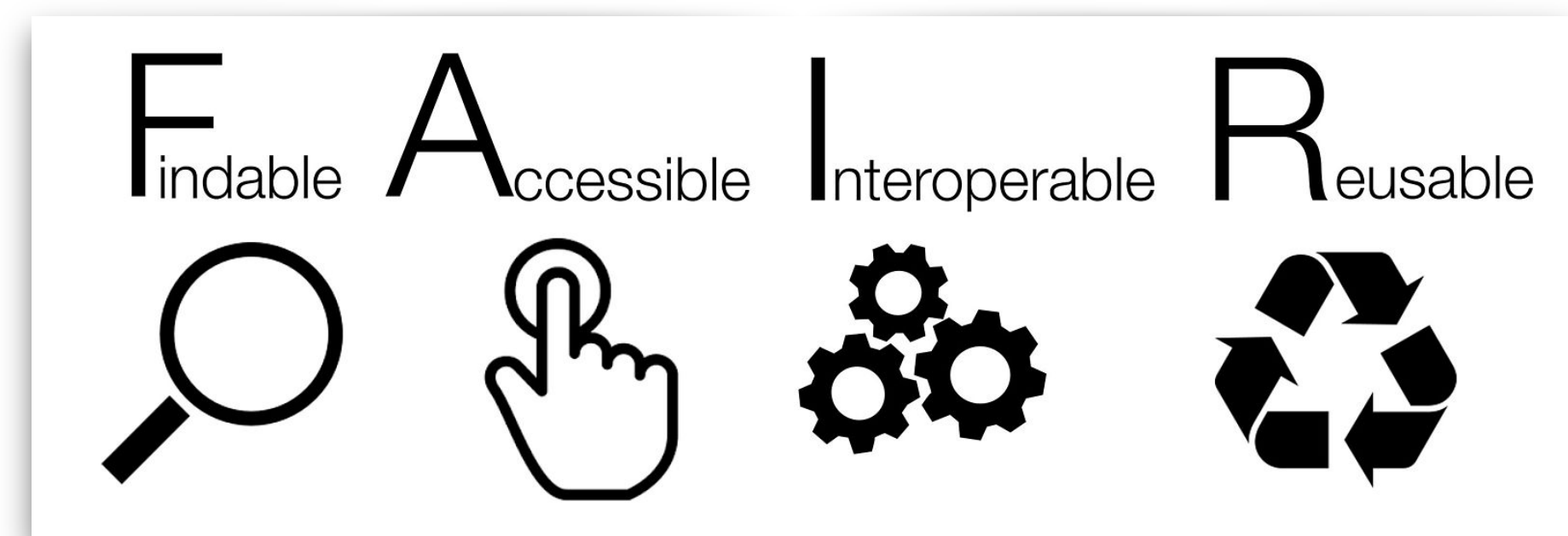
- + fluorescence method
- + imaging method
- + label free method
- luminescence method
 - alphascreen
 - bioluminescence
 - bioluminescence resonance energy transfer
 - **chemiluminescence**
 - chemiluminescence resonance energy transfer
- mass spectrometry
- + radiometry method



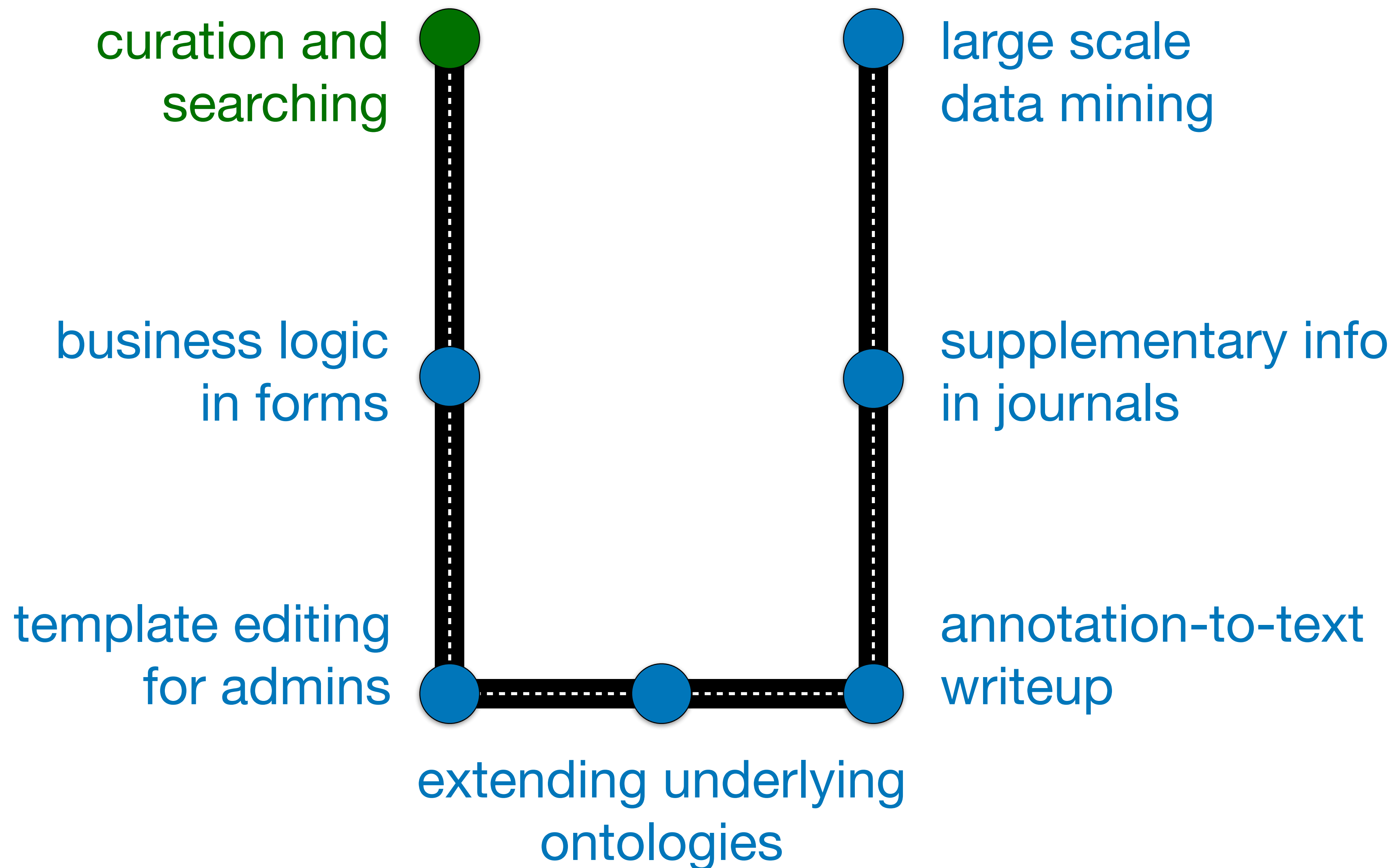


Collaboration

- ❖ Common terms: ontologies are universal
- ❖ Assays are directly comparable, regardless of source
- ❖ Interoperability:
 - ◆ reduce/eliminate ambiguity
 - ◆ share assays with CROs (and acquisitions)
 - ◆ preserve institutional knowledge
- ❖ Completeness: you know what you know...



Roadmap



Questions?



- ❖ Contact:

- ◆ Alex M. Clark alex@collaborativedrug.com (Collaborative Drug Discovery)

- ❖ Thanks to the Vault & BioAssay Express teams