



Building the BioAssay Research Database

A Next-Generation Platform for Annotating and
Understanding Chemical Biology Datasets

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Center for the Science of Therapeutics

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What is BARD?

A public platform for sharing chemical biology data that uses a standard representation and common language for organizing bioassays and their results.

Goal: To help researchers develop and test hypotheses on the influence of different probes on biological functions.

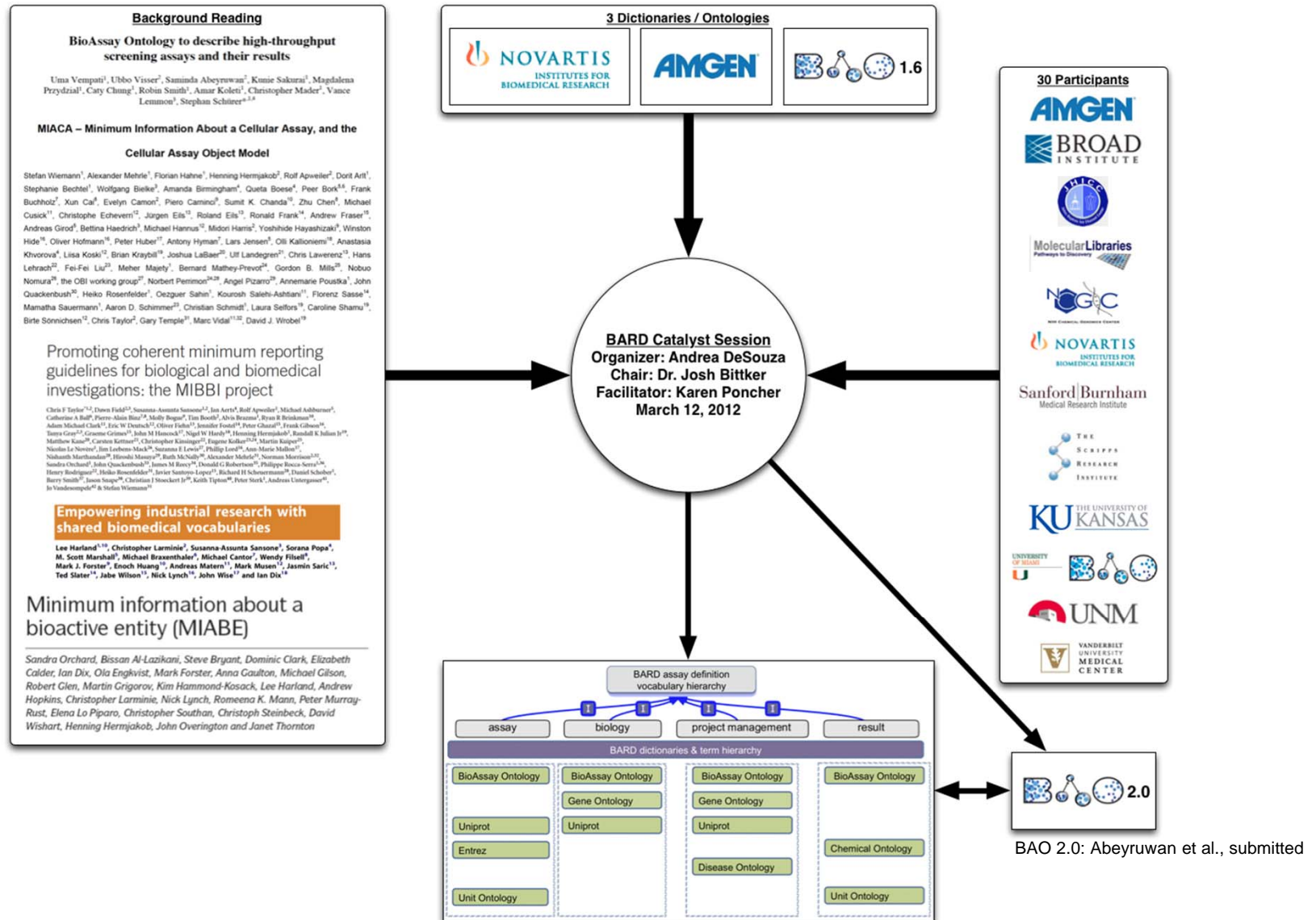
Precompetitive opportunities with BARD

- Standardized & controlled vocabulary to describe the context of experimental results
- Open source software platform to register assays, and to query and visualize public bioassay data
- An open standard for sharing bioassay annotations and data with the public or between organizations

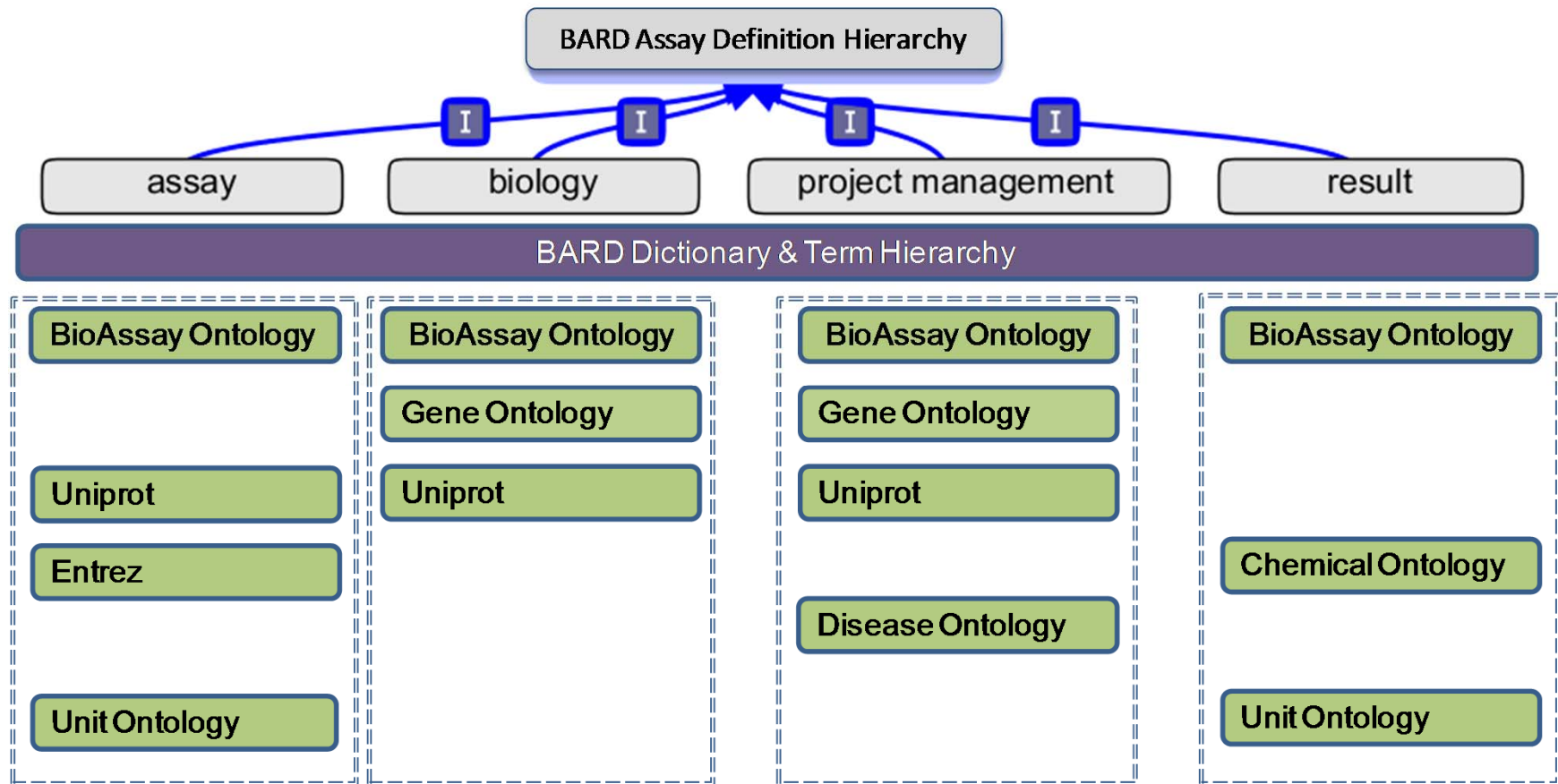
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Constructing a biologist-focused vocabulary



BARD top level concepts & sources



Curation of BARD-managed terms



Logged in as: jbittker

Empty

HOW TO ...

Propose New Term

1. Select a parent for

Selected Parent term:

assay kit name

Defined set of commercially available or well known materials, reagents and proven protocols needed for an assay to deliver concise results in the least amount of time. However, the specific molecular components may or may not be known (as in the case of proprietary kit components).

assay protocol > assay component > assay component type > assay kit name

Definition of selected parent term

Defined set of commercially available or well known materials, reagents and proven protocols needed for an assay to deliver concise

BARD Dictionaries

- assay component name
- assay kit name**
- assay provider name
- assay readout name
- assay reagent name
- clinical isolate name
- cultured tissue name
- detection instrument name
- experiment panel name
- instrument manufacturer name
- laboratory name
- other cell name
- project lead name
- project name
- RNA construct collection name
- screening campaign name
- small-molecule collection name
- tissue-culture flask name

Entire BARD Vocabulary

- No children can be added to this element
- Children can only be added through a request to the RDM Team
- Any user is allowed to add a child element and use the element immediately

☒ Do NOT show 'Retired' terms in hierarchy

- assay protocol
- biology
- project management
- result type

Curation of BARD-managed terms





SEARCH

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QUERY CART [Empty](#)


My BARD

[HOW TO ...](#) [SUPPORT](#)

Propose New Term (page 1 of 2)

1. Select a parent for your new term:

Selected Parent term:

 We set the parent term for you based on the attribute from your context item, however you can delete this and choose something else

Definition of selected parent term



Defined set of commercially available or well known materials, reagents and proven protocols needed for an assay to deliver concise

[Next: define term](#) [Close this window to cancel](#)

BARD Dictionaries

- assay component name
- **assay kit name**
- ACTOne Membrane Potential Dye Kit
- Adapta Universal Kinase Assay Kit
- ADP Hunter Plus Kit
- ADP-Glo Kinase Assay
- Alpcos insulin ELISA assay kit
- AlphaScreen Bead kit
- AlphaScreen Beads
- Amplex Red Glucos/Glucose Assay Kit
- ATPase Luminescence Assay System
- BacTiter-Glo Microbial Cell Viability Assay
- Beta-Glo Assay System
- BODIPY Nucleotide Analogue
- Bright-Glo Luciferase Assay System
- britelite plus Reporter Gene Assay System
- BTC AM Fluorescent Dye Indicator
- Calcium Assay Kit
- cAMP-Screen Direct System
- cash popper1 (Retired)
- Caspase-Glo 3/7 Assay System
- CDP-star
- Cell to CT RT kit
- CellTiter-Glo Luminescent Cell Viability Assay
- Chroma-Glo Luciferase Assay System
- CytoTox-ONE Homogenous Membrane Integrity Assay

Curation of BARD-managed terms



Logged in as: jbittker

Empty

HOW TO ...

Propose New Term (page 2 of 2)

Selected Parent term

Definition of selected parent term

2. Enter the name of your term and a definition for it. (both are required)

Proposed term *

Proposed definition *

3. Enter additional optional information about your term.

Abbreviation

Synonyms(Comma separated)

4. Explain why you need to add this term.

Explanation/Comments *

New terms are provisional but can be used immediately to avoid delays

Leveraging of external ontologies

Any updates to a referenced ontology are incorporated into BARD

SEARCH BARD Search assay, project and experiment data or [learn about BARD's innovative search features.](#)

erk1

erk1

erk1 as **Protocol**

erk1 and erk2 cascade as **GO Biological Process Term**

SEARCH

Desktop Client >

ERK1 and ERK2 cascade ; GO:0070371 [show def] [view in tree]

Symbol, full name	Information	Qualifier	Evidence	Reference	Assigned by
view associations AGT Angiotensinogen	BLAST protein from <i>Homo sapiens</i>	IEA With Ensembl:ENSRNOP00000024917		GO REF:0000019	Ensembl (via UniProtKB)
view associations AVP Vasopressin-neurophysin 2-copeptin	BLAST protein from <i>Homo sapiens</i>	IDA		PMID:18402937	UniProt (via UniProtKB)
view associations CCL11 Eotaxin	BLAST protein from <i>Homo sapiens</i>	IEA With Ensembl:ENSRNOP00000009756		GO REF:0000019	Ensembl (via UniProtKB)

Assay Definitions 0 Compounds 0 Projects 3

Showing 1-10 of 26 results

Assay ID	Assay Format	Assay Type	Detection Method Type	ADID	Name	Status
3730	cell-based format	second messenger assay	AlphaScreen	3730	qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay: Stimulation with EGF	Approved
4079	whole-cell lysate format	second messenger assay	AlphaScreen	4079	CounterScreen Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay	Approved
3520	cell-based format	second messenger assay	AlphaScreen	3520	qHTS Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay	Approved
4429	cell-based format	protein-small molecule interaction assay	confocal microscopy	4429	Image-Based HTS for Selective Antagonists for GPR55	Approved
1024	cell-based format	protein-small molecule interaction assay	fluorescence microscopy	1024	SAR Analysis for the identification of Selective Antagonists of GPR55 using an Image-Based Screen	Approved
723	cell-based format	protein-small molecule interaction assay	fluorescence microscopy	723	SAR Analysis of Selective Antagonists of GPR55 using an Image-Based Assay - Set 4	Approved
693	cell-based format	localization assay	fluorescence intensity	693	SAR Analysis of Selective Antagonists of GPR55 using an Image-Based Assay - Set 3	Approved
563	cell-based format	protein-small molecule interaction assay	fluorescence microscopy	563	SAR Analysis for the identification of Selective Agonists of GPR55 using an Image-Based Screen	Approved

All target-based screens that GO indicates are associated to the queried pathway (and phenotypic assays directly annotated with the pathway)

Leveraging of external ontologies

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Structure IDs erk1|

SEARCH

erk1

erk1 as Protocol

erk1 and erk2 cascade as GO Biological Process Term

ERK1 and ERK2 cascade ; GO:0070371 [show def] [view in tree]

Symbol, full name	Information	Qualifier	Evidence	Reference	Assigned by
<input type="checkbox"/> view associations AGT Angiotensinogen	BLAST protein from <i>Homo sapiens</i>	IEA With	Ensembl:ENSRNOP00000024917	GO REF:0000019	Ensembl (via UniProtKB)
<input type="checkbox"/> view associations AVP Vasopressin-neurophysin 2-copeptin	BLAST protein from <i>Homo sapiens</i>	IDA		PMID:18402937	UniProt (via UniProtKB)
<input type="checkbox"/> view associations CCL11 Eotaxin	BLAST protein from <i>Homo sapiens</i>	IEA With	Ensembl:ENSRNOP00000009756	GO REF:0000019	Ensembl (via UniProtKB)
<input type="checkbox"/> view associations CCR3 C-C chemokine receptor type 3	BLAST protein from <i>Homo sapiens</i>	IEA With	Ensembl:ENSRNOP00000008809	GO REF:0000019	Ensembl (via UniProtKB)

Assay Definitions (0) Compounds (0) Projects (3)

Showing 1-10 of 26 results

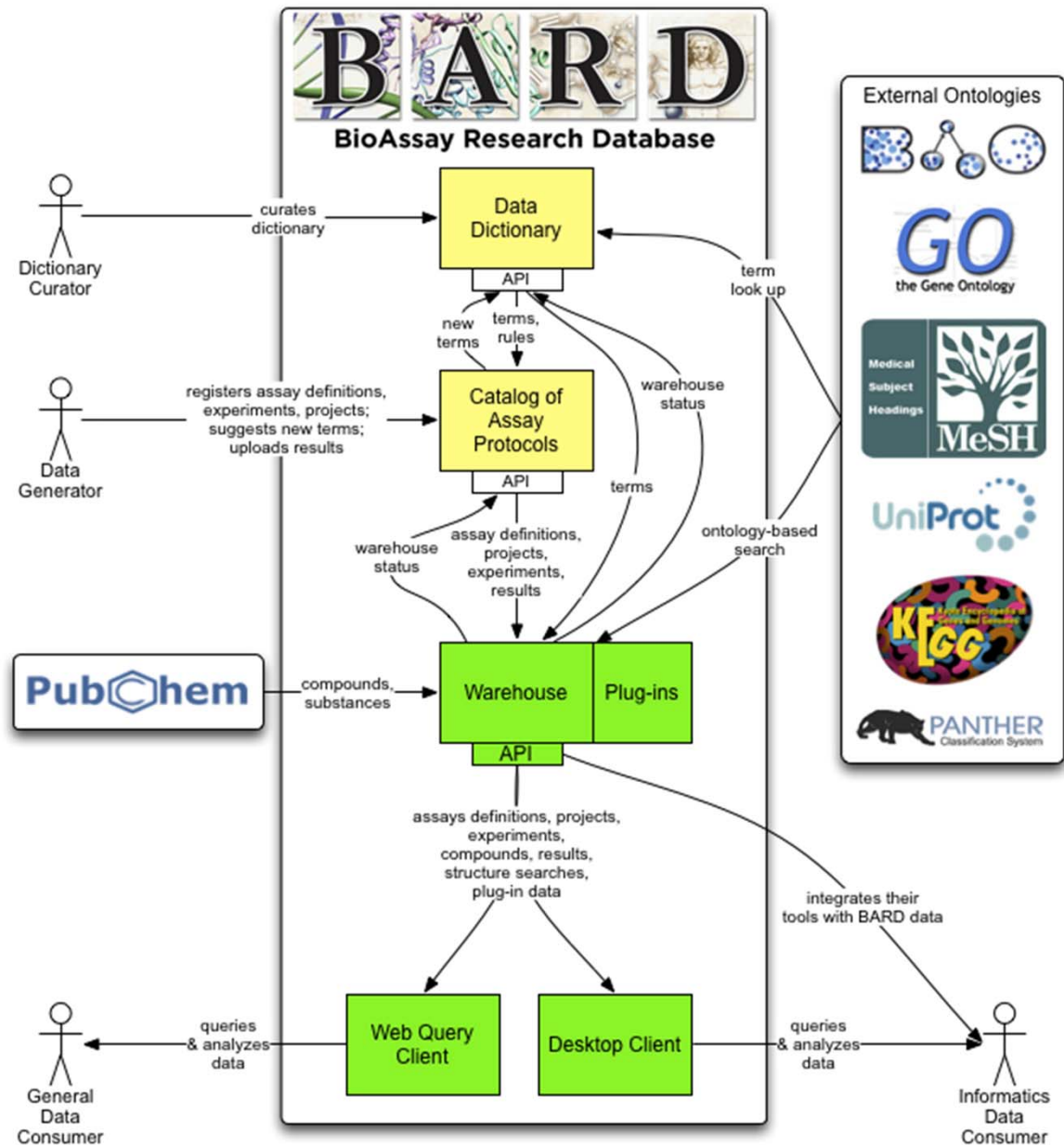
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New evidence added to GO is reflected in BARD search results

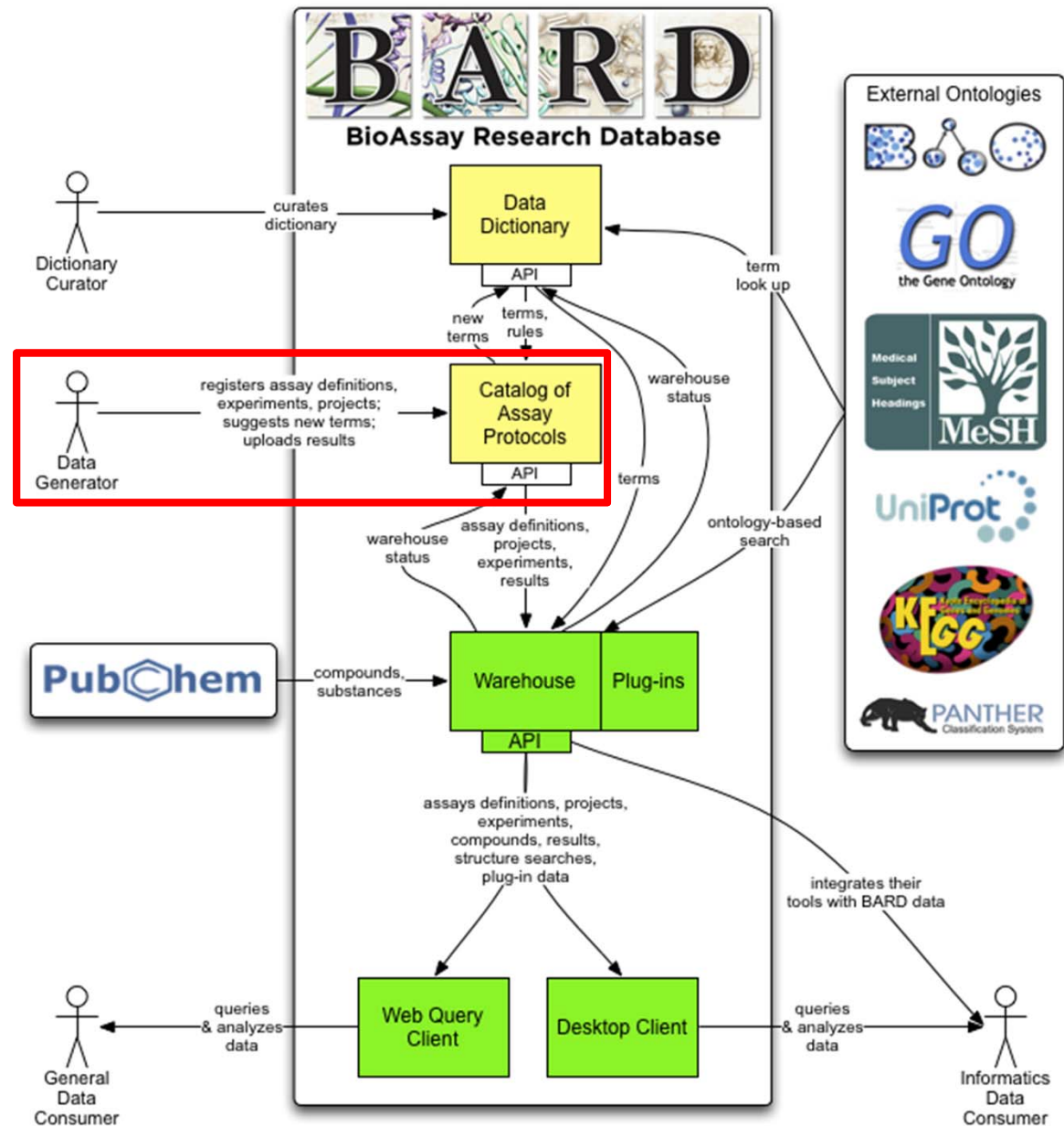
Precompetitive opportunities with BARD

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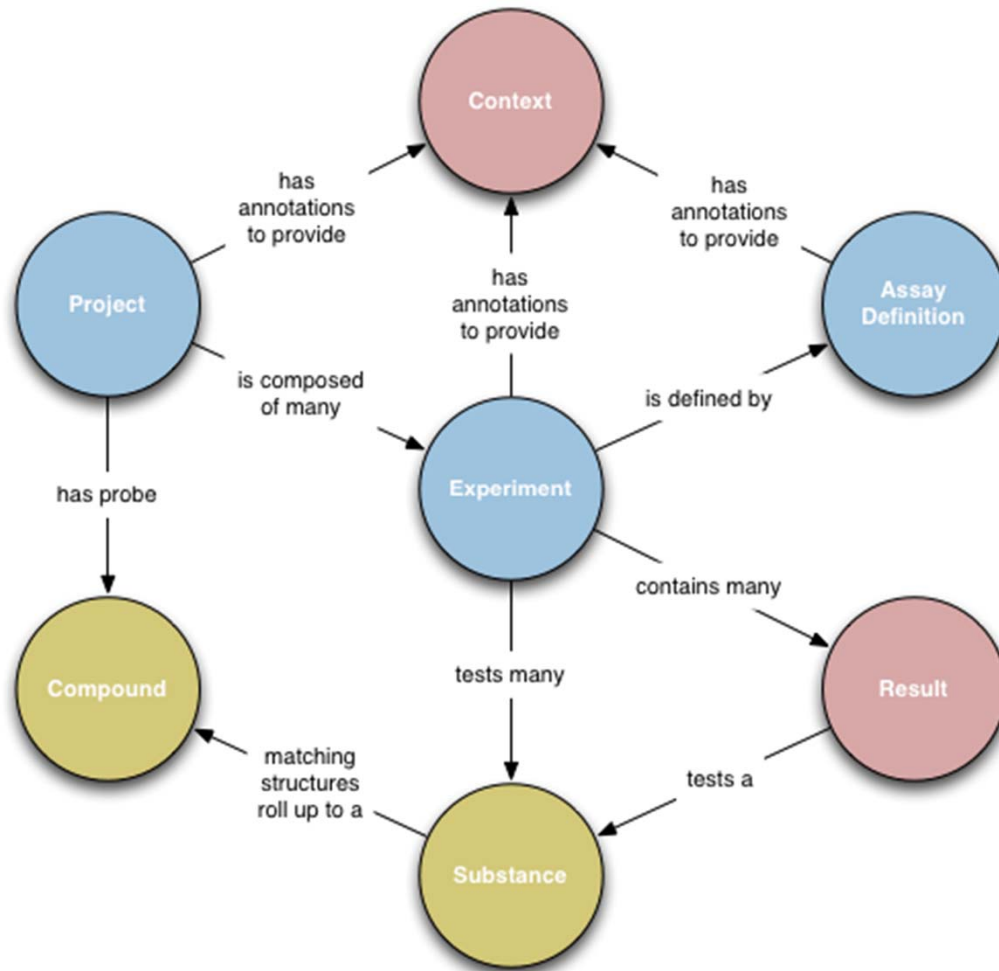
Build using component-based architecture






Build using component-based architecture



Structure for capturing bioassay relationships



-  Top-level entity: Organization
-  Data or metadata: System inputs
-  External identifiers

Interactive tools: assay definition

- Autocomplete & definitions for controlled terms

1. Overview	>
2. Biology	>
3. Assay Protocol	>
3.1. Assay Design	>
3.2. Assay Readout	>
3.3. Assay Components	>
3.4. Unclassified	>
4. Experiments	>
4.1. Experimental Variables	>
5. Documents	>
5.1. Descriptions	>
5.2. Protocols	>
5.3. Comments	>
5.4. Publications	>
5.5. External URLs	>
5.6. Others	>

2. Biology

biology	
<u>biology</u>	biological process
GO biological process term	(GO:0008219) cell death

Edit Biology

[Click here to view demo video on youtube](#)

3. Assay Protocol

assay format

Edit Assay Protocol

3.1 Assay Design

plate layout	
<u>assay footprint</u>	384-well plate

Edit Assay Design

Incubation time	
<u>incubation time</u>	1152.0 min

3.2 Assay Readout

assay readout	
<u>readout content</u>	single parameter
<u>readout type</u>	measured value
<u>readout signal direction</u>	signal decrease

Edit Assay Readout


detection method	
<u>detection instrument name</u>	PerkinElmer EnVision
<u>detection method type</u>	bioluminescence

measured component	
<u>assay component role</u>	measured component
<u>assay component name</u>	CellTiter-Glo Luminescent Cell Viability Assay

3.3 Assay Components

assay component	
<u>assay component role</u>	target cell
<u>assay component type</u>	cultured cell
<u>cultured cell name</u>	293

Interactive tools: projects



Structure IDs

SEARCH

Logged in as: jbittker Logout

QUERY CART Empty

My BARD

HOW TO ... SUPPORT

1. Overview

2. Annotations

3. Experiments and steps

4. Documents

4.1. Descriptions

4.2. Protocols

4.3. Comments

4.4. Publications

4.5. External URLS

4.6. Others

Project: Screen for RAS-Selective Lethal Compounds and VDAC Ligands Probe (Project ID: 907)

Ask a question about this Project

Save to Cart for analysis

1. Overview

PID: 907

Status: Approved

Name: Screen for RAS-Selective Lethal Compounds and VDAC Ligands

Description: Genetically matched immortalized cell lines expressing or not expressing HRAS-V12 were screened to identify compounds selectively lethal to cells expressing mutant HRAS. Two probe compounds, ML162 and ML210, were discovered.

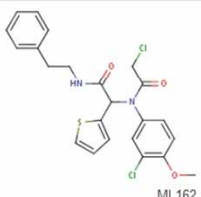
Owner: Broad Institute

Date Created: 05/19/2013

Last Updated: 01/14/2014

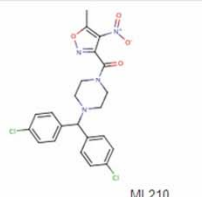
Modified By: sbrudz

Probes



Probe ML#: ML162


- Download probe report from Molecular Library BookShelf
- Show Compound Details in BARD
- View CID 3689413 in PubChem
- Show Experimental Details
- Show results for similar compounds tested in this project using %




Probe ML#: ML210

- Download probe report from Molecular Library BookShelf
- Show Compound Details in BARD
- View CID 49766530 in PubChem
- Show Experimental Details
- Show results for similar compounds tested in this project using %

[Click here to view demo video on youtube](#)

 **BROAD**
INSTITUTE

 **BARD**
BioAssay Research Database

Guided process for defining bioassays

- Suggests path for providing minimum information necessary to define an assay; Allows cloning & editing of existing public protocols

2. BIOLOGY

target

biology: macromolecule
amino acid substitution: HRas V12G

Edit Biology

3. ASSAY PROTOCOL

assay format

assay format: small-molecule format

Edit Assay Protocol

Completed

✓ Choose a biological process, biomolecule, or physio chemical property

✓ Specify the type of biomolecule and an identifier for it

✓ Specify an assay format

Next Steps

☐ Choose an assay type

☐ Choose detection method type

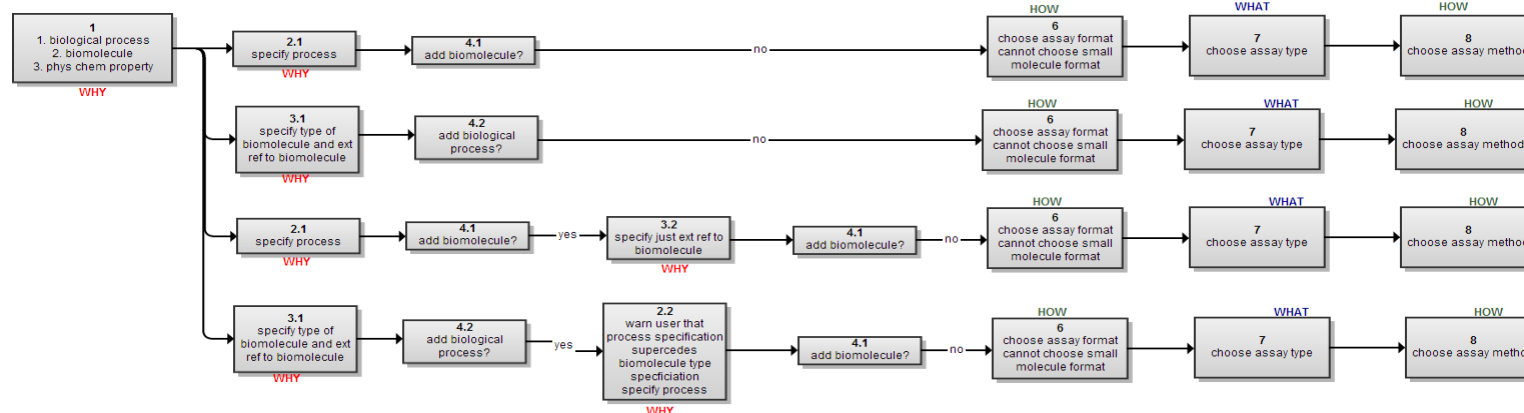
☐ Choose assay readout

☐ Specify at least one assay component

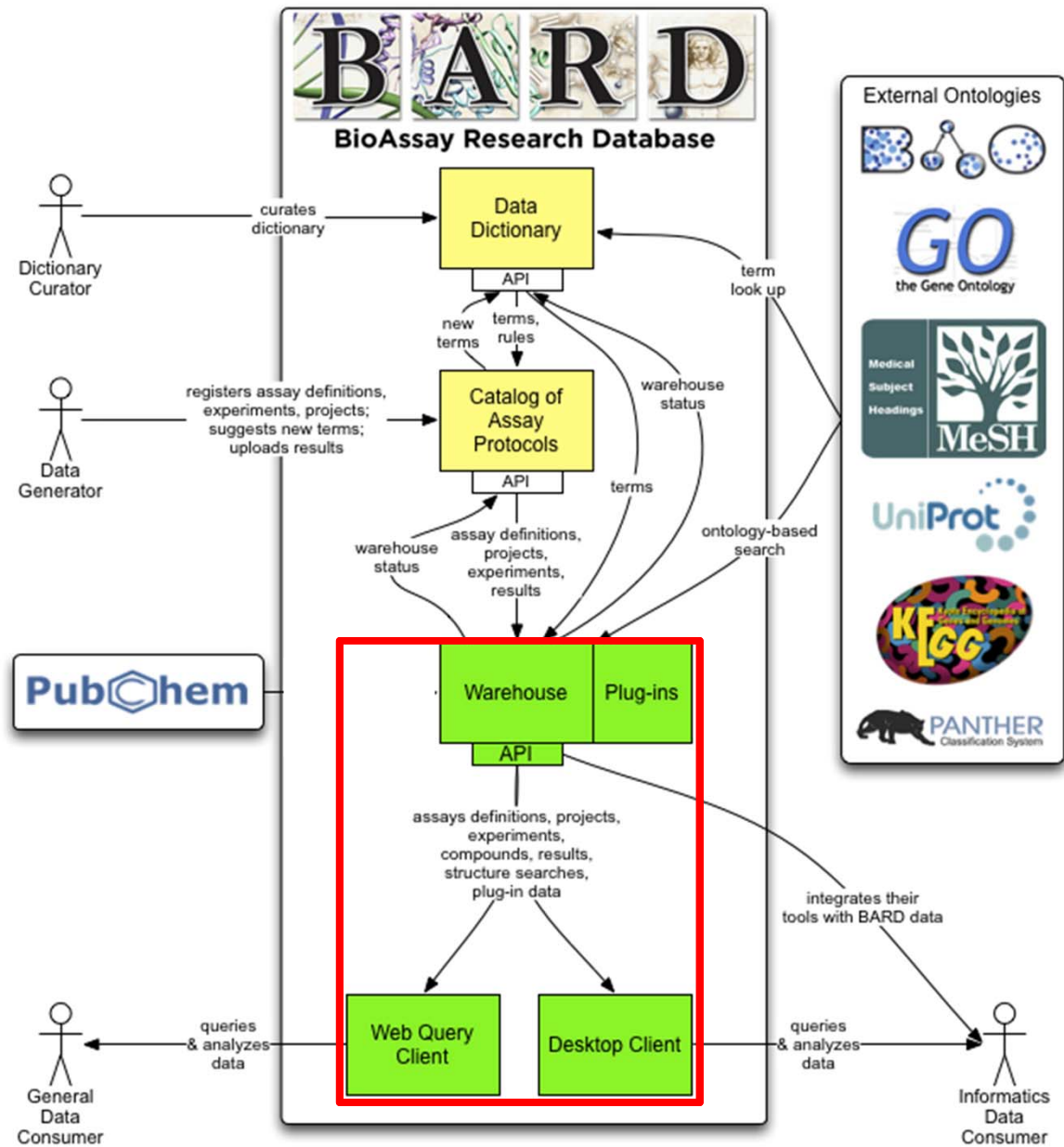
Warnings

⚠ You cannot specify both small-molecule format and a biology

- Logic checks for consistency



Using annotations: Finding & understanding bioassay data



Using annotations: Finding & understanding bioassay data

- Simple autocomplete interface allows basic searching by free text or specific annotation; searching by IDs or structures [Click here to view demo video on youtube](#)

The screenshot displays the BARD website. At the top, the BARD logo is on the left, and social media sharing buttons (Facebook, Twitter, LinkedIn, Google+) are in the center. On the right, it shows the user is logged in as 'jbittker' with a 'LOGOUT' button. Below the logo, the text reads 'Enhanced data and advanced tools to accelerate drug discovery.' and 'Introducing BARD, the powerful new bioassay database from the NIH Molecular Libraries Program. Now with unprecedented efficiency, scientists can develop and test hypotheses on the influence of different chemical probes on biological functions.' A 'LEARN MORE' button is present. The main section is titled 'SEARCH BARD' with a subtitle 'Search assay, project and experiment data or learn about BARD's innovative search features.' It features a search bar with 'Structure' and 'IDs' tabs, a 'SEARCH' button, and a link to 'Download the BARD Desktop Client'. Below this is a 'BARD NEWS' section with a tweet from David LaHr dated Jan 10 2014. The bottom section is titled 'Search and analyze your own way.' with the text 'Keeping the promise of the MLP, BARD gives you nimble access to most all the program's data through an array of query, analysis and visualization tools.' and a 'HOW TO VISUALIZE DATA' button. The background of the bottom section features a circular diagram with a chemical structure in the center and various assay types around it.

BARD
BioAssay Research Database

Enhanced data and advanced tools to accelerate drug discovery.

Introducing BARD, the powerful new bioassay database from the NIH Molecular Libraries Program. Now with unprecedented efficiency, scientists can develop and test hypotheses on the influence of different chemical probes on biological functions.

LEARN MORE

SEARCH BARD Search assay, project and experiment data or learn about BARD's innovative search features.

Structure IDs SEARCH

Download the BARD Desktop Client

BARD NEWS David LaHr - Jan 10 2014 @ 12:45 AM - BARD - helping you answer you answer Who, What, When, Where, Why and How about BioAssays

Search and analyze your own way.


Keeping the promise of the MLP, BARD gives you nimble access to most all the program's data through an array of query, analysis and visualization tools.

HOW TO VISUALIZE DATA

Using annotations: Finding & understanding bioassay data

- Filtering results allows a focus on the desired understanding: By target, assay details, reagent, etc.

[Click here to view demo video on youtube](#)



Structure IDs

gobp_term:"signal transduction"

SEARCH

Logged in as: jbittker Logout

QUERY CART Empty

My BARD

HOW TO ... SUPPORT

Assay Definitions 184 Compounds 2 Projects 23

Clear All Filters

Apply Filters

Filters

gobp_term

☒ "signal transduction"

Assay format

☐ cell-based format (119)

☐ biochemical format (23)

☐ single protein format (12)

☐ protein complex format (8)

[More](#)

Assay type

☐ protein-small molecule interaction assay (36)

☐ reporter-gene assay (31)

☐ protein-protein interaction assay (24)

☐ second messenger assay (18)

[More](#)

Detection method type

☐ fluorescence intensity (36)

☐ bioluminescence (25)

☐ chemiluminescence (21)

☐ fluorescence polarization (17)

[More](#)

Kegg disease category

☐ Cancer (26)

☐ Neurodegenerative disease (14)

☐ Endocrine disease (12)

☐ Developmental disorder (9)

[More](#)

Biological process

☐ positive regulation of extrinsic apoptotic signaling pathway (7)

☐ (go:0070493) thrombin receptor signaling pathway (6)

☐ (go:0030168) platelet activation (4)

☐ activation of cysteine-type endopeptidase activity involved in apoptotic process (4)

[More](#)

Target protein

☐ apoptosis regulator bcl-2 (7)

☐ induced myeloid leukemia cell differentiation protein mcl-1 (7)

☐ neurotensin receptor type 1 (7)

☐ tnfrsf10 tumor necrosis factor (ligand) superfamily, member 10 (7)

[More](#)

Showing 1-10 of 184 results

Add All	Assay Format	Assay Type	Detection Method Type	ADID	Name	Status
<input type="checkbox"/>	protein format	protein-protein interaction assay	fluorescence resonance energy transfer	3009	TR-FRET assay for 14-3-3 / Bad interaction inhibitors Matched Field: Description	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	biochemical format	enzyme activity assay	homogeneous time-resolved fluorescence	4081	Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay: MEK Inhibition Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	cell-based format	signal transduction assay	absorbance	2540	ELISA Cell-Based Counter Assay to Identify Inducers of cAMP in Platelets Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	cell-based format	signal transduction assay	bioluminescence	3433	Confirmation Concentration-Response Assay for Cell signaling CRE-BLA (Fsk stim) - HEK293 CREB Luciferase Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	biochemical format	enzyme activity assay	homogeneous time-resolved fluorescence	4075	Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay: EGFR T790M/L858R Kinase Inhibition Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	biochemical format	enzyme activity assay	homogeneous time-resolved fluorescence	4077	Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay: c-Raf Inhibition Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	single protein format	direct enzyme activity assay	homogeneous time-resolved fluorescence	4076	Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay: EGFR L858R Kinase Inhibition Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	single protein format	direct enzyme activity assay	homogeneous time-resolved fluorescence	4078	Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay: EGFR T790M Kinase Inhibition Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	whole-cell lysate format	second messenger assay	AlphaScreen	4079	Counterscreen Assay for Inhibitors of the ERK Signaling Pathway using a Homogeneous Screening Assay Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved
<input type="checkbox"/>	cell-based format	functional assay	fluorescence intensity	3441	Confirmation Concentration-Response Assay for Cell signaling CRE-BLA (Fsk stim) Matched Field: Dictionary Value	<input checked="" type="checkbox"/> Approved

Previous 1 2 3 4 5 6 7 8 9 10 ... 19 Next

Visualizing data using structured annotations

- Filtering and visualizing activity allows rapid understanding of multiple datasets

BARD BioAssay Research Database

Logged in as: jbittker Logout

Structure IDs ML162 SEARCH QUERY CART Empty My BARD

HOW TO ... SUPPORT

ML162 Probe

(PubChem CID: 3689413)

[Click here to view demo video on youtube](#)

☐ Save to Cart for analysis

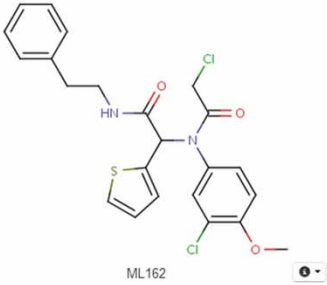
Bio-activity Summary Linked Hierarchy Visualization

Assays - Active vs Te... **24 / 101**

IUPAC Name: 2-{3-chloro-N-(2-chloroacetyl)-4-methoxyanilino}-N-(2-phenylethyl)-2-thiophen-2-ylacetamide
Probe ID: ML162
Project ID: 907
• View Probe by CID (3689413) in PubChem

SMILES: COC1=C(C)C=C(C=C1)N(C(C(=O)NCCC2=CC=CC=C2)C3=CC=CS3)C(=O)CCl

Molecular Weight: 477.403
Exact Mass: 476.073
Rotatable Bonds: 9
HBond Acceptors: 4
HBond Donors: 1
LogP: 5.2
Total Polar Surface ... 86.9



ML162

Scaffold Promiscuity Analysis

Scaffold	Count	Action
	285	Show details
	142	Show details
	115	Show details
	61	Show details
	23	Show details

PubChem Substances

5066159 17509717 40211455 50291668 87342575 87692475 89856179 92709052 99222866 99351092 99495782 103162096 103162097 104543588 112137762 125044172 126273328 136936835 140105829

About: History, Development Team
Help: Forums, Submit a Bug Report, Ask a Question
Technology: Architecture & Design, REST API, Source code on GitHub, **Calling card**
RDM: Organizing principles, Top-level concepts, Glossary

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Scitelligence
© 2013 BARD

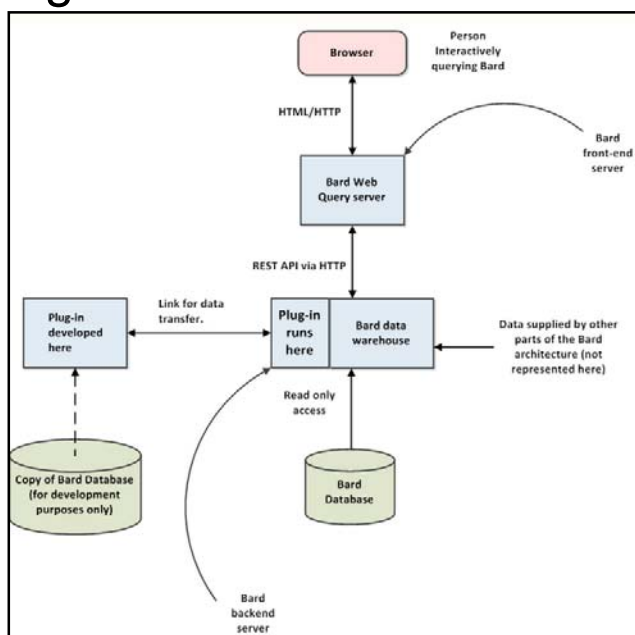
By using BARD, you agree to our [terms of use](#) and [privacy policy](#)
Release created: Thu Dec 19 22:47:23 EST 2013 Branch: iteration.039.0 Revision: da7ee99c1c5fe45ac4cc9aacdfa56e53d3788e36

Additional uses of annotations

- Establishing a measure of similarity between assays to enable clustering of protocols

ADID 3431: Cell Viability - CRE-beta lactamase CHO cell - 24 hr assay		ADID 3432: Cell Viability - CRE-beta lactamase CHO cell - 40 hr assay	
Cards unique to ADID: 3431		Cards unique to ADID: 3432	
assay conditions		assay conditions	
incubation time	1440.0 min	incubation time	2400.0 min
assay format		assay design	
assay format	cell-based format	assay method	viability measurement method
detection method		counterscreen	compound toxicity assay
assay method	viability measurement method	viability measurement method	ATP quantitation
viability measurement method	ATP quantitation	assay type	
detection method type	luminescence method	assay format	cell-based format
target cell		assay type	viability assay
assay component role	target cell	target cells	
cultured cell name	CHO	assay component role	target cell
expressed protein	reporter gene	cultured cell name	CHO
species name	Cricetulus griseus	species name	Cricetulus griseus

- Plugin architecture allows direct calls to warehouse API for metadata



Name	Lead Author[s]	Institution	Brief Description	Status
Badapple	Jeremy Yang	UNM	Evidence-based promiscuity scores	released Oct 2012
SmartCyp	Rajarshi Guha	NCGC	Prediction of which sites in a molecule that are most liable to metabolism by Cytochrome P450	released March 2013
WhichCyp	Rajarshi Guha	NCGC	Prediction of which Cytochrome P450 isoform(s) is(are) likely to bind a drug-like molecule	released June 2013
HScaf	Jeremy Yang	UNM	Scaffold analysis	In development
TBE (kNN)	Oleg Ursu	UNM	kNN, nearest neighbors bioactivity profiler	In development
TBE (Filtering)	Jeremy Yang	UNM	Druglike/leadlike/probelike suitability filtering	In development
Assay based similarity	Vlado Dancik	Broad	Compound similarity based on bioactivity	In development
TBE (SVM)	Lars Carlsson & UNM	AstraZeneca	SVM classifier	Planned
ALOGPS	Igor Tetko	HZM & UNM	LogP prediction	Planned
TBE (QSAR)	Alex Tropsha	UNC & UNM	QSAR modeling	Planned

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Sharing bioassays using a common language

- Controlled vocabulary with public references

230	high-signal control	BARD> assay protocol> assay component> assay component role> assay definition role> assay control role> high-signal control Contains the substrate titration without inhibitor to reflect the maximum enzyme activity at each substrate concentration. Depending on the composition of the inhibitor stocks, DMSO might be needed in the control wells to assure consistency across all the experiments.	BioAssay Ontology : http://www.bioassayontology.org/bao#BAO_0000156
231	low-signal control	BARD> assay protocol> assay component> assay component role> assay definition role> assay control role> low-signal control Contains the substrate titration without enzyme or substrate and without inhibitor. The low controls should reflect the signal expected for no enzyme activity at each substrate concentration. Depending on the composition of the inhibitor stocks, DMSO might be needed in the control wells to assure consistency across all the experiments.	BioAssay Ontology : http://www.bioassayontology.org/bao#BAO_0000168
232	negative control	BARD> assay protocol> assay component> assay component role> assay definition role> assay control role> negative control Used to determine the baseline against which the effect of the test perturbagen is compared. Often the negative control is the solvent (e.g., DMSO) in which the perturbagen was dissolved.	BioAssay Ontology : http://www.bioassayontology.org/bao#BAO_0000079
233	positive control	BARD> assay protocol> assay component> assay component role> assay definition role> assay control role> positive control A chemical compound or reagent used in each plate of an assay to normalize the response of the test perturbagens (by plate). The positive control is known from previous experiments or is a previously established standard. It is usually highly active, resulting in a strong response of the intended effect. In an inhibition assay, the positive control would usually result in the complete inhibition, which measurement is then used for normalization. In an activation assay it would result in high activation, which measurement is then used for normalization. Using controls provides an external reference and reduces the number of false negatives and false positives.	BioAssay Ontology : http://www.bioassayontology.org/bao#BAO_0000080
151	cell-culture role	BARD> assay protocol> assay component> assay component role> assay definition role> cell-culture role	
249	antibiotic	BARD> assay protocol> assay component> assay component role> assay definition role> cell-culture role> antibiotic	Open Biomedical Ontologies - CHEBI : http://purl.obolibrary.org/obo/CHEBI_22582
250	differentiation agent	BARD> assay protocol> assay component> assay component role> assay definition role> cell-culture role> differentiation agent	BioAssay Ontology : http://www.bioassayontology.org/bao#BAO_0002087
251	fixative	BARD> assay protocol> assay component> assay component role> assay definition role> cell-culture role> fixative	Open Biomedical Ontologies - CHEBI : http://purl.obolibrary.org/obo/CHEBI_50913

- Business rules: what is required to minimally define an assay?

2. Biology ³

biology

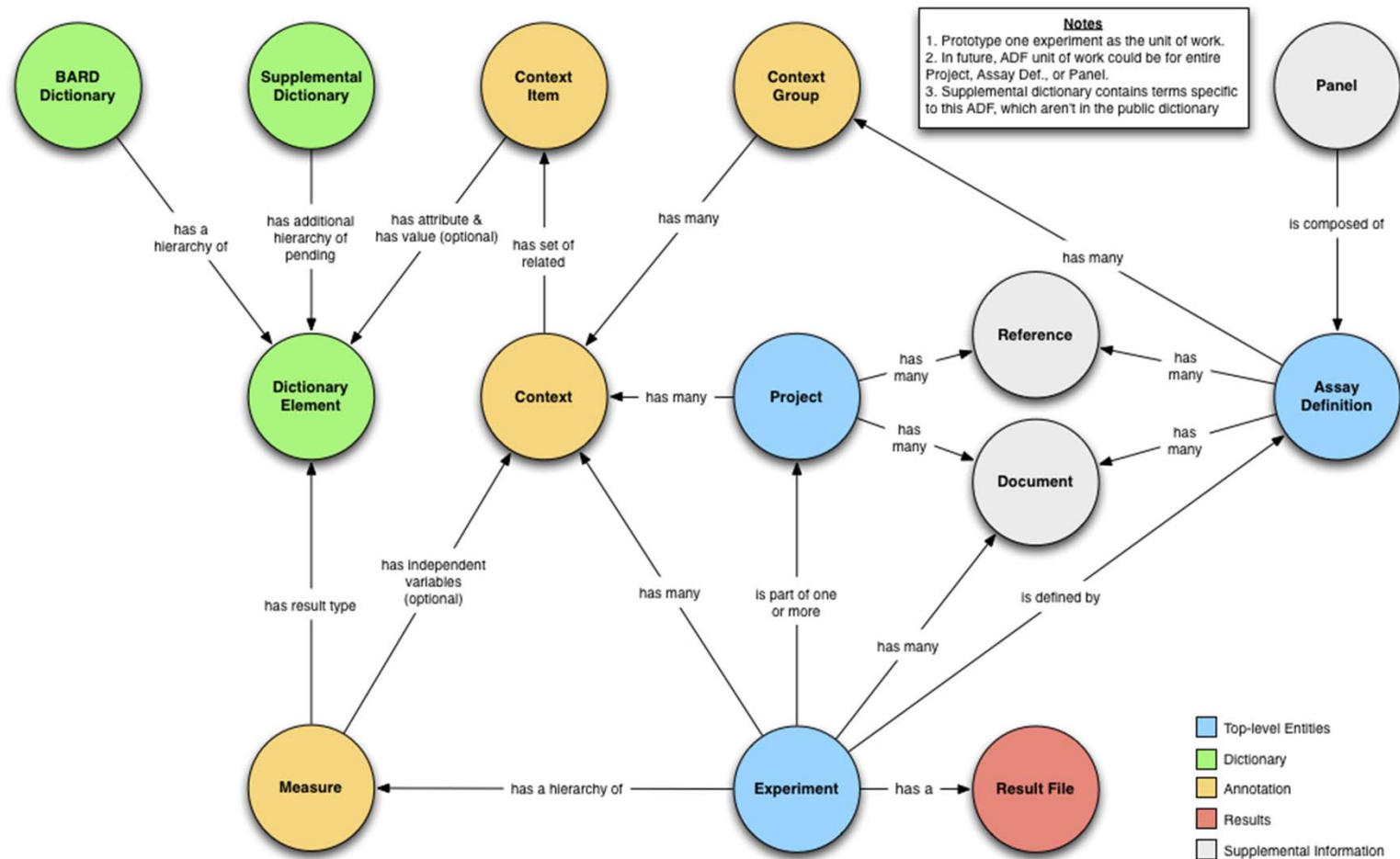
biology

macromolecule

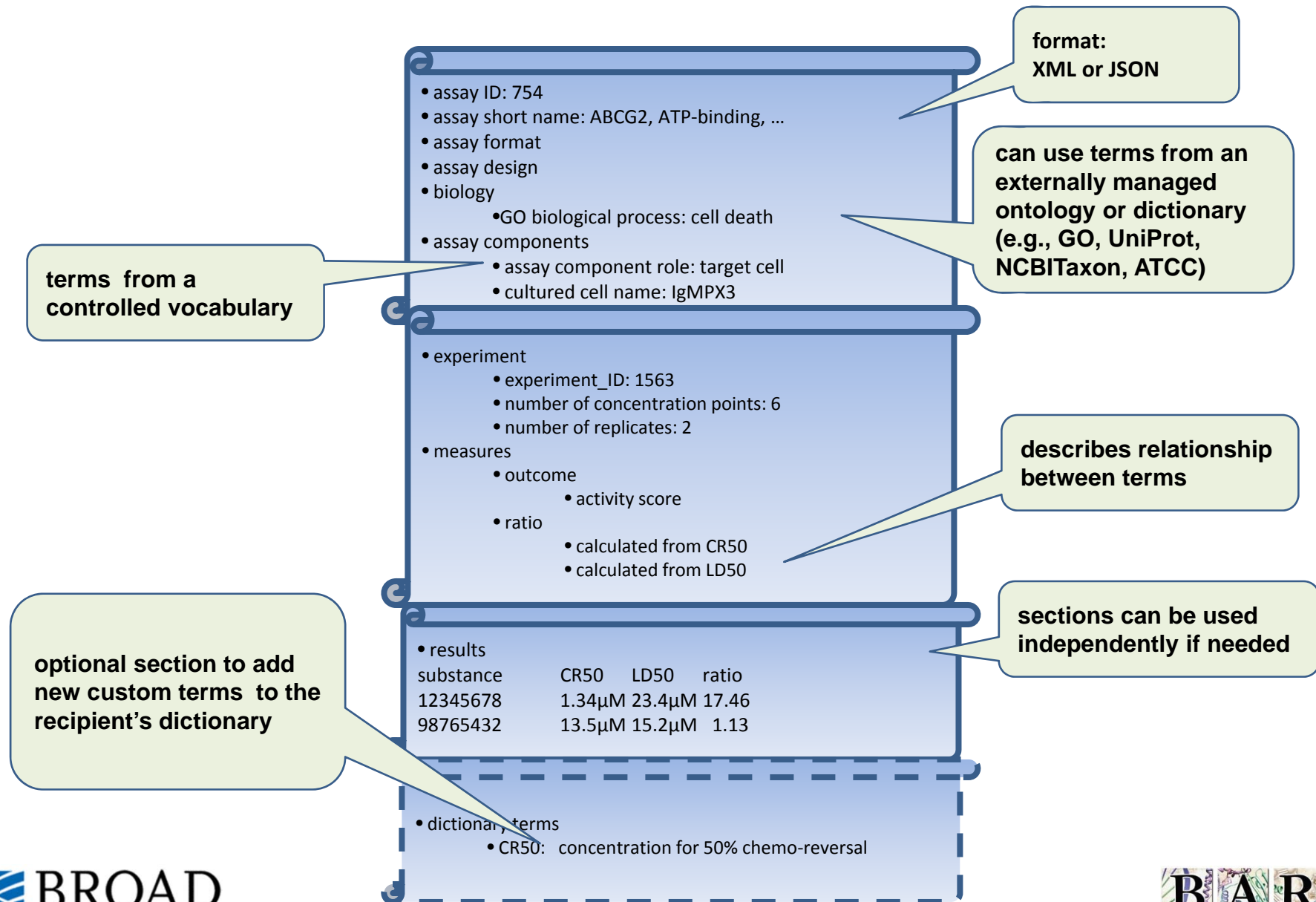
- When a context has biology defined as a something that can be considered a molecular target, there should one other item that references one of the following terms (GO gene-product ID, GenBank ID, NCBI accession number, UniProt accession number, gene Entrez GI, protein Entrez GI).

- Object relational structure

Formalizing object relationships





Assay Definition Format



Using with private data

- User ID: Currently Atlassian Crowd, changing to Mozilla Persona
- Objects owned by teams, editable by users on team
- Desktop client allows direct import of private structures and assays, including encrypted structure transfer for comparison to public data store

Compound	Class	Name	Active/Texted ...	IUPAC
 NCGC00241363-01		NCGC00241363-01		
 NCGC00241364-01	Screening Compound	NCGC00241364-01	2/93	N-(3...
 NCGC00241364-01	Screening Compound	NCGC00241365-01	0/91	N-(3...
 NCGC00241365-01	Patent Compound	NCGC00187213-01	0/6	N-(3...
 NCGC00187213-01	Screening Compound	NSC00234222	0/91	7-(di...
 NSC00234222	ML Probe	NCGC00333223-01	5/9	N-(4...
 NCGC00333223-01				

- Private deployments- open source code and documentation for creating internal build. 3rd party licenses required: Oracle, ChemAxon

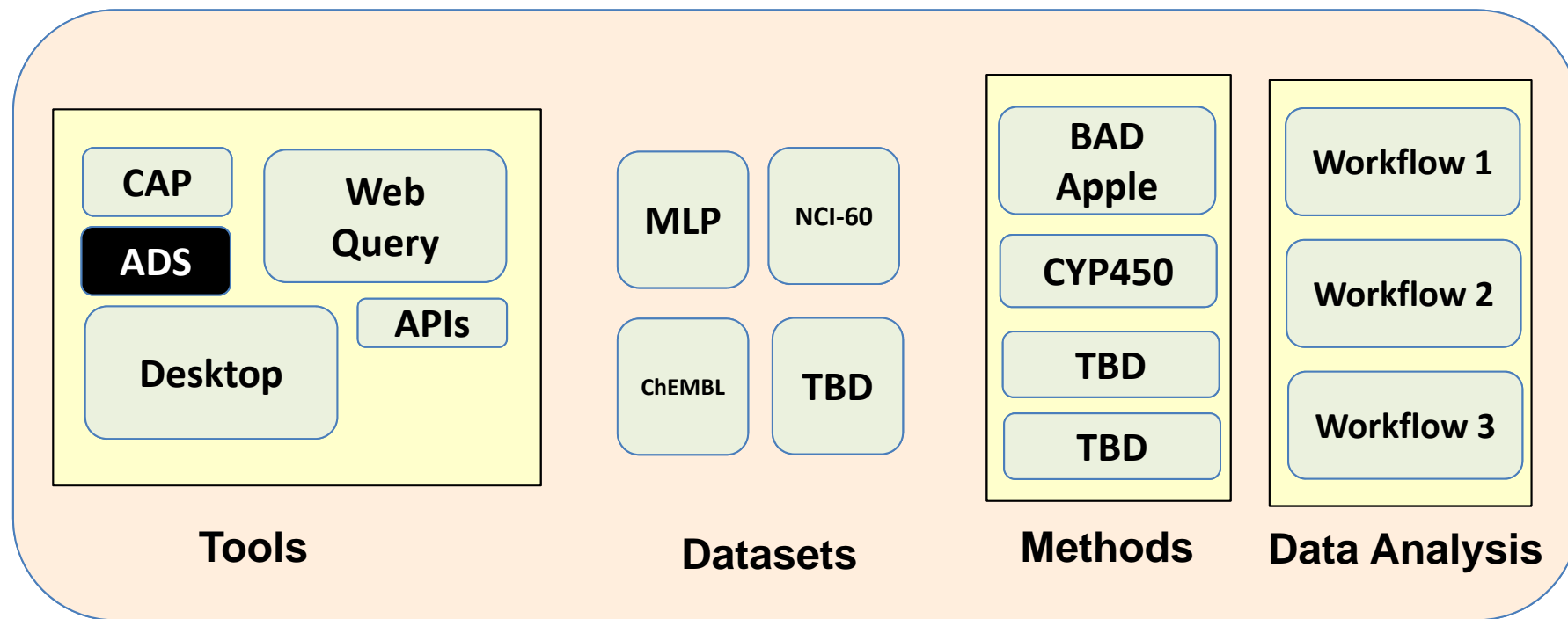
Upcoming improvements

- Query tools public, demonstrations on BioAssay Research Database YouTube channel
- Annotation tool release Feb 2014
- Addition of public datasets beyond MLP including signature-based data e.g. LINCS
- Release of additional plugins
- Normalization of chemical names and structures to further standardize data

Long-Term Path Forward



as a Platform



Sustained Community Engagement

<http://bard.nih.gov>

Direct Contributors



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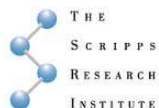
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