

# Screensaver User Manual

Screensaver is an open source, web based *Laboratory Information Management System* (LIMS) developed at and used by the ICCB-Longwood Screening Facility (ICCB-L). Screensaver first launched in June 2007. A revised, updated version of Screensaver launched in December 2018. Screensaver supports the storage and comparison of screening datasets, as well as the management of information about screens, screeners, libraries and laboratory work requests.

Screensaver access is restricted to ICCB-L screeners with an active Small Molecule or RNAi User Agreement on file.

## ***A few helpful points to keep in mind:***

Since there is so much information available in Screensaver, not all data is displayed by default. The **Add columns**, **Add other screen columns** and **Add study column buttons** on the left side of tables can be selected to modify the displayed columns. Check the box next to the information you would like included in the table.

Magnifying glass icons located above some columns enables querying information within a specific column. Sorting and nested sorting of table columns is possible in Screensaver. By default, columns with numeric values are sorted low to high and columns with strings are sorted alphabetically. To sort a column, click on the column's title. An icon with the sort order # and arrow indicating the direction of sort is displayed. To perform a nested sort, click the title of the next column to be sorted.

Each page in Screensaver has a unique URL. This provides a convenient way of relaying information to colleagues with Screensaver access or ICCB-L team members should any issues or questions arise.

You can navigate through Screensaver using the forward and back buttons in your web browser. If you have advanced past a page of interest and would like to get back to it, use the back button on your web browser. Using the tabs within Screensaver will revert to default conditions as opposed to options you may have selected.

When exporting data, only columns that are visible in the viewable table are included. Prior to downloading, confirm that all columns of interest are displayed in the table.

## ***Examples within:***

Example 1 (page 3): Determine the molecular weight range of compounds within a library.

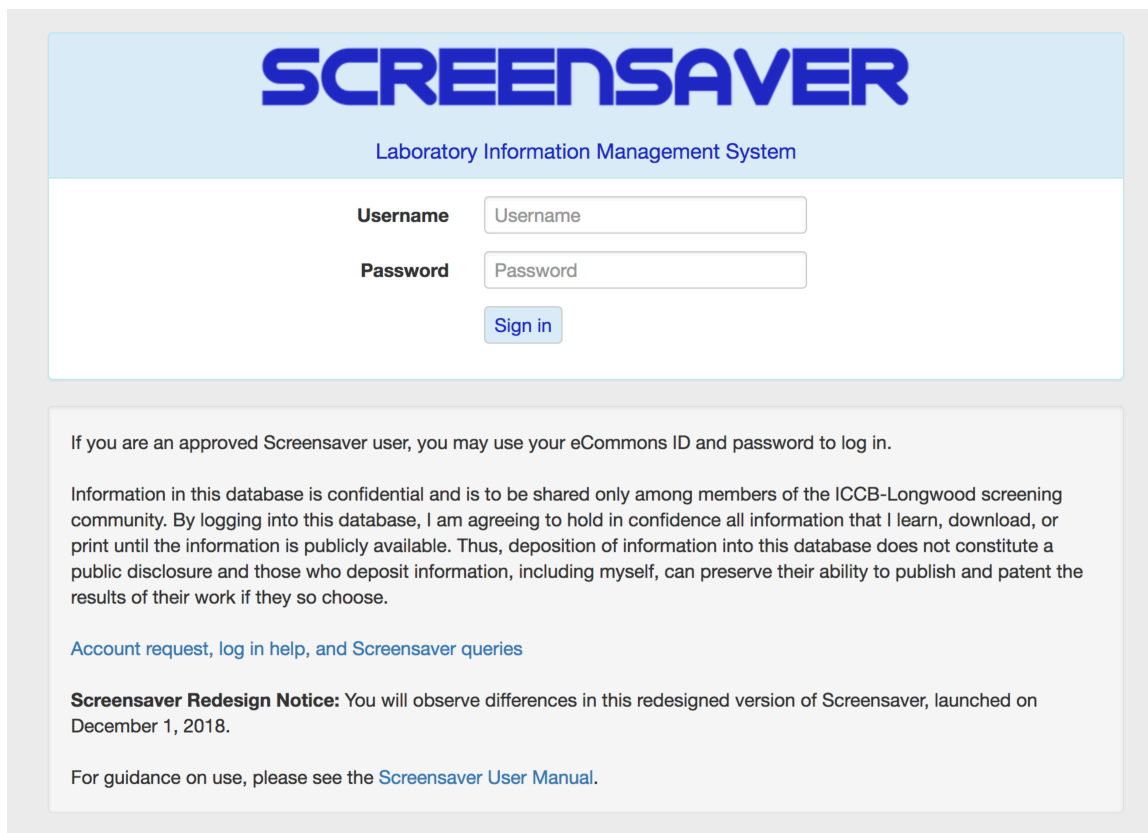
Example 2 (page 5): Identify which small molecule libraries contain compounds that target EGFR.

Example 3 (page 7): Download a file of all potential hits identified in User's screen, including columns for compound structure and compound ID.

Example 4 (page 10): View compound name and structure for a particular plate and well location (or multiple wells).

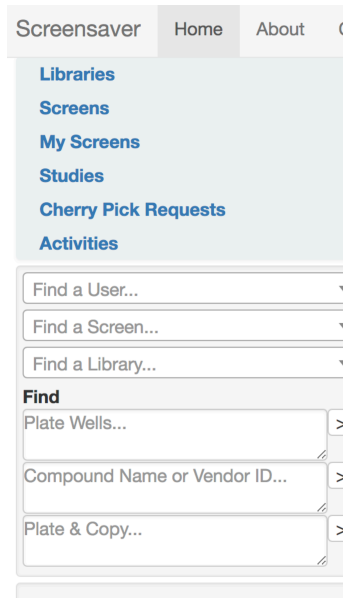
## Getting started:

To sign in, go to the Screensaver sign page (<https://screensaver.med.harvard.edu>) and enter your eCommons ID and password, then click **Sign in**.



The image shows the login page for the Screensaver Laboratory Information Management System. At the top, the word "SCREENSAVER" is displayed in large blue letters, with "Laboratory Information Management System" written below it in a smaller font. The login section contains two input fields: "Username" and "Password", each with a placeholder text of the same name. Below these fields is a blue "Sign in" button. A paragraph of text below the login section states: "If you are an approved Screensaver user, you may use your eCommons ID and password to log in." Another paragraph follows, explaining the confidentiality of the database and the user's agreement to hold information in confidence. Below this is a link: "Account request, log in help, and Screensaver queries". A "Screensaver Redesign Notice" is also present, stating that the system was redesigned and launched on December 1, 2018. Finally, a link to the "Screensaver User Manual" is provided for guidance on use.

The home page will appear. Screensaver provides three options for accessing data: 1) menu navigation; 2) text search with autofill; and 3) Find text search. Clicking on **Screensaver** in the horizontal search bar will return you to this Home page.



The image shows the home page of the Screensaver system. At the top, there is a navigation bar with "Screensaver", "Home", and "About" links. Below this is a vertical menu with the following items: "Libraries", "Screens", "My Screens", "Studies", "Cherry Pick Requests", and "Activities". Below the menu are three search input fields: "Find a User...", "Find a Screen...", and "Find a Library...". Below these is a "Find" section with three input fields: "Plate Wells...", "Compound Name or Vendor ID...", and "Plate & Copy...". Each of these three input fields has a magnifying glass icon to its right. At the bottom of the page, there is a horizontal search bar.



## Menu Navigation

**Libraries**  
**Screens**  
**My Screens**  
**Studies**  
**Cherry Pick Requests**  
**Activities**

Clicking on each of the categories will display:

**Libraries:** Information on individual small molecule and RNAi libraries.

**Screens:** List of all screens User has permission to view. This is dependent upon the user agreement on file and selected data sharing level.

**My Screens:** A list of all screens User has conducted or collaborated on at ICCB-L.

**Studies:** ICCB-L compiles information on libraries that many investigators will find helpful during data analysis and follow up experiments. These include studies on compound fluorescence, toxicity, target information and frequency of hits in screens conducted at ICCB-L.

**Cherry Pick Requests:** A list of User's cherry pick requests.

**Activities:** A list of all activities conducted by User and their collaborators (when associated with a screen) at ICCB-L. This includes training, library screening, cherry pick screening and custom automation. To see only User activities, click on **User's name**, then **Activities** tab.

*Searching via the menu is particularly useful when querying an entire category, for example viewing particular items within an entire library or screen.*

### **Example 1. Determine the molecular weight range of compounds within a library.**

Select **Libraries**, then **Small Molecule Libraries**. Libraries appear alphabetically and you can scroll to the one of interest.

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logged in as: ghf

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RNAi Libraries

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Find a Screen...

Find a Library...

Find

Plate Wells...

Compound Name or Vendor ID...

Plate & Copy...

Clear searches

Add columns

Page 1 of 1 pages, 93 Small Molecule Libraries

Download

Rows500

Short Name	Experimental Well Count	Provider	Plate Size	Library Type	Screening Status	Start Plate	End Plate	Plate Count
ActiMolTimTec1	8,517	Biomol-TimTec	384	Commercial	Allowed, Requires Permission	1534	1558	25
Asinex1	12,378	Asinex	384	Commercial	Allowed	1671	1706	36
Asinex 2	23,031	Asinex	384	Commercial	Allowed	3769	3840	72
Asinex 3	3,923	Asinex	384	Commercial	Allowed	3841	3853	13
Belfer Frag 1	3,000	ChemBridge	384	Fragment	Requires Permission	3695	3703	9
Biomol4	640	Biomol	384	Known Bioactives	Allowed	2089	2090	2
BiomolICCBL-2012	480	Enzo Life Sciences	384	Known Bioactives	Allowed	3402	3403	2
BiomolICCBL-2017	470	Enzo Life Sciences	384	Known Bioactives	Allowed	3854	3855	2
Biomol-XuTan	0	Enzo Life Sciences	384	Known Bioactives	Allowed	3642	3643	2
Bionet2	1,700	Bionet	384	Commercial	Allowed	1364	1368	5
BMABE1	351	Clardy Lab, HMS	384	Natural Products	Requires Permission	3876	3876	1
BU-CMD 2017	2,457	BU-CMD	384	Academic Collection	Requires Permission	3762	3768	7
Cayman Biolipid 1	831	Cayman Chemical	384	Known Bioactives	Allowed	3648	3650	3
CB GPCR	250	ChemBridge	384	Known Bioactives	Allowed	3407	3407	1
CB IONCore	250	ChemBridge	384	Known Bioactives	Allowed	3408	3408	1
CB KINACore	250	ChemBridge	384	Known Bioactives	Allowed	3410	3410	1

**Alternative:** enter library name in the autofill Find a Library... text search.

Click on the library short name (eg Selleck-10mM) to view.

Screensaver Home About Contact

**Libraries**

- Small Molecule Libraries
- RNAi Libraries
- All Active and Retired Libraries

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**Studies**

**Cherry Pick Requests**

**Activities**

Find a User...  
Find a Screen...  
Find a Library...

**Find** ?

Plate Wells... >

Compound Name or Vendor ID... >

Plate & Copy... >

Library: Selleck-10mM

Library Details **Wells**

<b>Short Name:</b>	Selleck-10mM
<b>Library Name:</b>	Selleck Bioactive Compound Library - 10mM
<b>Experimental Well Count:</b>	1,902
<b>Provider:</b>	Selleck Chemicals
<b>Screen Type:</b>	Small Molecule
<b>Plate Size:</b>	384
<b>Solvent:</b>	DMSO
<b>Library Type:</b>	Known Bioactives
<b>Pool:</b>	False
<b>Screening Status:</b>	Allowed
<b>Start Plate:</b>	3651
<b>End Plate:</b>	3657
<b>Plate Count:</b>	7
<b>Description:</b>	-
<b>Version Number:</b>	2
<b>Is Archived:</b>	False

Click **Wells**, then **Add columns**. You will see columns that can be displayed. Check the boxes next to all information you would like displayed and uncheck the box for any information you are not interested in viewing. Click **Continue** and the table will be updated.

Select Columns to display

Continue Cancel and return to page

**Available Columns**

Search... Q Clear Collapse

- ☒ Reagent
  - ☐ Comment
  - ☐ Vendor Batch ID
  - ☒ Vendor Reagent ID
  - ☒ Vendor
- ☐ Report
  - ☐ Other Wells With Reagent
- ☒ SmallMoleculeReagent
  - ☐ ChEMBL IDs
  - ☒ Compound Name(s)
  - ☐ InChI
  - ☐ Restricted
  - ☐ Molecular Formula
  - ☐ Molecular Mass
  - ☒ Molecular Weight
  - ☐ PubChem CIDs
  - ☐ SMILES
  - ☐ Structure Image
- ☒ Well
  - ☐ Deprecation Reason
  - ☐ Facility ID
  - ☐ Deprecated
  - ☐ Library Full Name
  - ☒ Library
  - ☒ Library Well Type
  - ☒ Concentration (mg/ml)
  - ☐ Molar Concentration
  - ☒ Plate
  - ☐ Screen Type
  - ☐ Well ID
  - ☒ Well

**Selected Columns**

Unselect

- ☒ Reagent
  - ☒ Vendor Reagent ID
  - ☒ Vendor
- ☒ SmallMoleculeReagent
  - ☒ Compound Name(s)
  - ☒ Molecular Weight
- ☒ Well
  - ☒ Library
  - ☒ Library Well Type
  - ☒ Concentration (mg/ml)
  - ☒ Plate
  - ☒ Well

Cancel and return to page Continue

Click on **Molecular Weight** to sort from high to low.

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**Libraries**

Small Molecule Libraries

RNAi Libraries

All Active and Retired Libraries

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Find a User...

Find a Screen...

Find a Library...

**Find**

Plate Wells...

Compound Name or Vendor ID...

Plate & Copy...

Library: Selleck-10mM

Library Details Wells

Clear sorting Add columns Add study columns Add screen columns

Page 1 of 112 pages, 2688 Small Molecule Residants Download Rows 24

Plate	Well	Library	Library Well Type	Molar Concentration	Vendor	Vendor Reagent ID	Molecular Weight	Compound Name(s)
3651	C05	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S1214	1512.622290000	Bleomycin Sulfate
3652	A22	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S4146	1408.666740000	Bacitracin
3655	O20	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S1902	1355.365180000	Vitamin B12
3651	C21	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S1832	1243.479180000	Atracurium Besylate
3655	H19	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S2113	1243.479180000	Cisatracurium Besylate
3651	O14	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S2199	1219.588800000	Aliskiren Hemifumarate
3651	F20	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S3073	1213.417040000	Caspofungin Acetate
3653	N15	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S7597	1205.573440000	BV-6
3654	L18	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S1514	1202.611240000	Cyclosporine
3651	O16	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S2286	1202.611240000	Cyclosporin A
3655	H17	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S2077	1155.341720000	Atorvastatin Calcium
3652	N08	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S4286	1140.236910000	Anidulafungin (LY303366)
3652	H06	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S4269	1079.105940000	Vinorelbine Tartrate
3651	J09	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S2637	1067.265640000	TAK-875
3652	I07	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S3162	1066.186920000	Tylosin tartrate
3652	B17	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S4227	1058.039160000	Fidaxomicin
3654	A11	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S1044	1030.287080000	Temsirolimus (CCI-779, NSC 683864)
3652	F03	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S4163	1025.874720000	Doxycycline Hyclate

If you wish to view or manipulate the data in another program (eg Excel, Vortex, KNIME), click **Download** to export the data. Prior to downloading, confirm all desired columns are visible. Only columns displayed in the table will be downloaded. Available formats for export are xlsx, csv and sdf.

### Example 2. Identify which small molecule libraries contain compounds that target EGFR.

In the menu, select **Studies**, then **100010** (Vendor-provided compound description/activity/target).

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Find a User...

Find a Screen...

Find a Library...

**Find**

Plate Wells...

Compound Name or Vendor ID...

Plate & Copy...

**100010: Vendor-provided compound description/activity/target**

Study Details Data

**Date Recorded:** -

**Library Screen Type:** Small Molecule

**Study ID:** 100010

**Title:** Vendor-provided compound description/activity/target

**Lab Name:** Shamu, Caroline - Harvard Medical School, ICCB-L (HMS)

**Lab Affiliation:** Harvard Medical School, ICCB-L (HMS)

**Lead Screener:** David Wrobel

**Study Type:** In silico

**Summary:** Chemical vendor-provided annotations of compounds within ICCB-Longwood known bioactive libraries that includes: functional class descriptions, biological/pharmacological activities, therapeutic uses, and/or protein targets (enzyme inhibitors and activators; receptor antagonists and agonists). Note that ICCB-Longwood staff have not curated the information content nor confirmed its accuracy. Also, this study does not summarize all known bioactivity information available in the scientific literature for each compound. This information can be supplemented with additional PubChem data that are available for most known bioactive compounds by clicking on the CID link in the well view for each in Screensaver. David Wrobel (ICCB-Longwood) updated this data in Screensaver July 2018.

**Homepage:** -

**Comments:**

**Collaborators:**

Select **Data**, then the **magnifying glass icon** in the Vendor-provided compound description/activity/target column. Search type is set to 'contains' and 'EGFR' is entered into the search box. Click **Ok**.

ScreensaverHomeAboutContactlogged in as: ghfLog out

LibrariesScreensMy ScreensStudiesCherry Pick RequestsActivities

Find a User...Find a Screen...Find a Library...FindPlate Wells...Compound Name or Vendor ID...Plate & Copy...

100010: Vendor-provided compound description/activity/target

Study DetailsData

Reagent AnnotationsData Columns

Add columnsAdd screen columnsAdd other study columns

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DownloadRows25

Plate	Well	Library	Library Well Type	Reagent Vendor	Vendor Reagent ID	Compound Name(s)	Vendor-provided compound description / activity / target [100010]
1920	A03	NINDS2	Experimental	NINDS	1500101	Acetaminophen	analgesic, antipyretic; synthetic
1920	A04	NINDS2	Experimental	NINDS	1500201	Cloxacillin sodium	antibacterial; semisynthetic
1920	A05	NINDS2	Experimental	NINDS	1500102	Acetazolamide	carbonic anhydrase inhibitor, diuretic, antiglaucoma; synthetic
1920	A06	NINDS2	Experimental	NINDS	1500202	Cloxyquin	antibacterial, antifungal; synthetic
1920	A07	NINDS2	Experimental	NINDS	1500103	Acetohydroxamic acid	urease inhibitor, antitumor, antibacterial; synthetic
1920	A08	NINDS2	Experimental	NINDS	1500205	Colchicine	antimitotic, antitumor agent; Colchicum autumnale
1920	A09	NINDS2	Experimental	NINDS	1500104	Acetylcholine	antitachycardic, miotic, vasodilator (peripheral); synthetic
1920	A10	NINDS2	Experimental	NINDS	1500206	Colistimethate sodium	antibacterial; Bacillus colistinus

The updated table will contain a list of all experimental wells in which the vendor has indicated EGFR as a target.

ScreensaverHomeAboutContactlogged in as: ghfLog out

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Find a User...Find a Screen...Find a Library...FindPlate Wells...Compound Name or Vendor ID...Plate & Copy...

100010: Vendor-provided compound description/activity/target

Study DetailsData

Reagent AnnotationsData Columns

Clear searchesAdd columnsAdd other study columns

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DownloadRows25

Plate	Well	Library	Library Well Type	Reagent Vendor	Vendor Reagent ID	Compound Name(s)	Vendor-provided compound description / activity / target [100010]
3229	C05	EMD1	Experimental	EMD Biosciences	203696	BPIQ-I	A potent and specific inhibitor of the tyrosine kinase activity of the epidermal growth factor receptor (EGFR; IC50 = 25 pM); Rewcastle, G.W., et al. 1996. J. Med. Chem. 39, 918.
3229	C09	EMD1	Experimental	EMD Biosciences	234505	Compound 56	The most potent and specific inhibitor of the tyrosine kinase activity of the EGFR (IC50 = 6 pM); Bridges, A.J., et al. 1996. J. Med. Chem. 39, 267.
3229	C21	EMD1	Experimental	EMD Biosciences	324673	EGFR/ErbB-2 Inhibitor	A potent, reversible inhibitor of EGFR and c-erbB2 (IC50 = 20 nM & 79 nM, respectively), members of the type I growth factor receptor family; Cockerill, S., et al. 2001. Bioorg. Med. Chem. Lett. 11, 1401.
3229	E03	EMD1	Experimental	EMD Biosciences	324674	EGFR Inhibitor	A potent, and highly selective inhibitor of EGFR and some EGFR mutants (IC50 = 21 nM, 63 nM, and 4 nM for EGFRwt, EGFRL858R and EGFRL861Q, respectively) vs. erbB4/Her4 (IC50 = 7.64 μM) and a panel of 55 other kinases; Zhang, Q., et al. 2006. J. Am. Chem. Soc. 128, 2182
3229	G21	EMD1	Experimental	EMD Biosciences	448101	Met Kinase Inhibitor	A potent, reversible inhibitor of Met kinase activity (IC50 = 20 nM). Exhibits > 60-fold selectivity over Fik and > 400-fold selectivity over Ron, FGFR-1, c-Src, Cdk2, PDGFRb, EGFR, and Tie-2; Ma, P. C., et al. 2005. Cancer Res. 65, 1479. Berthou, S., et al. 2004. Oncogene 23, 5387. Wang, X., et al. 2003. Mol. Cancer Ther. 2, 1085. Sattler, M., et al. 2003. Cancer Res. 63, 5462.
3229	I03	EMD1	Experimental	EMD Biosciences	513035	PD 158780	A potent inhibitor of the EGFR tyrosine kinase activity (IC50 = 8 pM); Cunick, J.M., et al. 1998. J. Biol. Chem. 273, 14468. Rewcastle, G.W., et al. 1998. J. Med. Chem. 41, 742.
3229	I05	EMD1	Experimental	EMD Biosciences	513040	PD 174265	A potent reversible, and selective inhibitor of EGFR tyrosine kinase activity (IC50 = 450 pM); Fry, D.W., et al. 1998. Proc. Natl. Acad. Sci. USA 95, 12022.
3229	K03	EMD1	Experimental	EMD Biosciences	529574	PP3	A negative control compound for the Src family protein tyrosine kinase inhibitor PP2 (Cat. No. 529573). However, it inhibits the activity of EGFR kinase (IC50 = 2.7 μM); Traxler, P., et al. 1997. J. Med. Chem. 40, 3601.

November 2018

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**Example 3. Download a file of all potential hits identified in User's screen, including columns for compound structure and compound ID.**

In the search menu, select **My Screens**. A list of all screens you conducted or collaborated on at ICCB-L are displayed.

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Screensaver Libraries Screens **My Screens** Studies Cherry Pick Requests Activities Reports

Find a User... Find a Screen... Find a Library... Find Plate Wells... Compound Name or Vendor ID... Plate & Copy...

Screen

Select columns

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Download Rows 25

Screen ID	Screen Type	Lab Head	Lab Affiliation	Lead Screener	Title	Status	Status Date	Screen Result
1238	Small Molecule	Bing Chen	Boston Children's Hospital (HMS Affiliated Hospital)	Gary Frey	Inhibit the binding of the envelope glycoprotein HIV gp41 to its target	Completed	05/10/2017	Available
150	Small Molecule	Stephen Harrison	Harvard Medical School, BCMP Department (HMS)	Gary Frey	Disrupt formation of the fusion-competent conformation of GP-41, an HIV coat protein.	Completed	05/22/2007	Available

Click **Screen ID #** of interest.

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Libraries Screens **Small Molecule Screens** RNAi Screens **My Screens** Studies Cherry Pick Requests Activities

Find a User... Find a Screen... Find a Library... Find Plate Wells... Compound Name or Vendor ID... Plate & Copy...

Screen Status: Completed

1238: A screen for compounds that... Inhibit the binding of the envelope glycoprotein HIV gp41 to its target

Screen Details Screening Summary Protocol Cherry Picks Activities Data

Screen ID: 1238  
Screen Type: Small Molecule  
Lab Name: Chen, Bing - Boston Children's Hospital (HMS Affiliated Hospital)  
Lead Screener: Gary Frey  
Title: Inhibit the binding of the envelope glycoprotein HIV gp41 to its target  
Status: Completed  
Status Date: 05/10/2017  
Collaborators: (David) O'Neil Danis, Jiwon Ha  
Summary: A screen for compounds that inhibit the binding of the envelope glycoprotein HIV gp41 to its target. An FP assay has been developed and the positive control will be an excess of unlabeled protein. Hits will be those compounds that disrupt gp41 binding to its target.  
Assay Type: Biochemical  
Screen Sharing: Data Sharing Level: Level 3 (Private)  
Assay Readout Types: FP  
Screen Result: Available  
Screening Count for Experimental Wells (Non-unique): 169,786

Activity Summary

Activities 54

Last Activity Date 2016-03-31  
Activity Type Informatics  
Performed By Dave Wrobel

Recent Cherry Pick Requests (Total: 6)

#	Date Requested	Requested By
44400	2016-01-04	Gary Frey
44384	2015-10-16	Gary Frey
44376	2015-09-14	Gary Frey
44377	2015-09-14	Gary Frey
44364	2015-07-14	Gary Frey
44274	2014-03-03	Gary Frey

The **Screening Summary** tab provides more detailed information, including the option to view all **Plates Screened** and **Libraries Screened**. The protocol provided in the primary screen report can be viewed by clicking **Protocol**. Any cherry picks requests and the corresponding plate maps can be viewed by clicking **Cherry Picks**. A summary of all activities associated with the screen, including training, library screening, external library screening and cherry pick transfers, is found in **Activities**. To view deposited data, click **Data**.

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Screen Status: Completed
1238: A screen for compounds that... Inhibit the binding of the envelope glycoprotein HIV gp41 to its target
Screen Details
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Screen Results
Data Columns
Add columns
Add other screen columns
Add study columns
Show positive rows only
Mutual positives
Download
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Rows 25

Plate	Well	Library	Library Well Type	Reagent Vendor	Vendor Reagent ID	Compound Name(s)	Assay Well Control Type	Fluorescence Polarization_A [1238]	PChannel_A [1238]	SChannel_A [1238]	Fluorescence Polarization_B [1238]	PChannel_B [1238]	SChannel_B [1238]	Z-score_A [1238]	Z-score_B [1238]	Z-score_Avg [1238]
587	A01	ChemDiv1	Experimental	ChemDiv	000A-0001			53.1	19,022,030	19,041,809	53.4	19,722,086	19,751,772	-0.2	0.32	0.06
587	A02	ChemDiv1	Experimental	ChemDiv	0180-0395			50.9	19,099,719	19,033,428	51.1	20,157,583	20,095,993	0.21	0.74	0.48
587	A03	ChemDiv1	Experimental	ChemDiv	000A-0193			51.6	18,670,665	18,630,271	56.2	19,030,265	19,167,465	0.08	-0.2	-0.06
587	A04	ChemDiv1	Experimental	ChemDiv	0272-0044			47.9	18,634,673	18,457,972	47.4	19,544,755	19,340,252	0.77	1.43	1.1
587	A05	ChemDiv1	Experimental	ChemDiv	000A-0285			49.9	18,457,914	18,357,156	52.1	18,873,348	18,853,635	0.4	0.56	0.48
587	A06	ChemDiv1	Experimental	ChemDiv	0310-0113			49.6	18,266,105	18,155,682	55.2	18,403,268	18,500,069	0.46	-0.02	0.22
587	A07	ChemDiv1	Experimental	ChemDiv	000A-0389			51.4	18,063,427	18,018,703	55.6	18,358,013	18,466,989	0.12	-0.09	0.01
587	A08	ChemDiv1	Experimental	ChemDiv	0337-0600			49.6	18,381,664	18,269,538	54.8	18,876,203	18,959,276	0.46	0.06	0.26
587	A09	ChemDiv1	Experimental	ChemDiv	000A-0533			50.3	18,664,590	18,578,564	53	19,120,989	19,133,252	0.32	0.39	0.36
587	A10	ChemDiv1	Experimental	ChemDiv	0389-0798			51.6	18,353,288	18,313,565	51.6	18,927,013	18,887,766	0.08	0.65	0.37
587	A11	ChemDiv1	Experimental	ChemDiv	000A-0692			50.1	18,618,248	18,524,426	56.6	18,733,155	18,884,387	0.36	-0.28	0.04
587	A12	ChemDiv1	Experimental	ChemDiv	0423-0162			51.9	17,220,761	17,196,263	55.6	17,379,034	17,483,449	0.02	-0.09	-0.03
587	A13	ChemDiv1	Experimental	ChemDiv	000A-0804			49.6	18,600,910	18,488,800	51.5	18,996,318	18,952,620	0.46	0.67	0.56
587	A14	ChemDiv1	Experimental	ChemDiv	0467-0868			48	19,584,333	19,402,004	51.9	19,049,194	19,021,492	0.76	0.59	0.67

All results are displayed. Depending upon the number of data columns, the table may continue out of view to the right. To only display potential hits, select the box next to **Show positive rows only**.

Often, investigators find it useful to include additional information, including compound SMILES, structure images, PubChem CIDs, etc. Click **Add columns** to modify what is displayed. When all columns to be displayed are selected, click **Continue**.

Continue
Cancel and return to page

Select Columns to display

Available Columns
Search...
Clear
Collapse

Reagent
Comment
Vendor Batch ID
Report
Other Wells With Reagent
Screenresult-1238
Fluorescence Polarization\_A [1238]
PChannel\_A [1238]
SChannel\_A [1238]
Fluorescence Polarization\_B [1238]
PChannel\_B [1238]
SChannel\_B [1238]
Z-score\_A [1238]
Z-score\_B [1238]
Z-score\_Avg [1238]
Criteria1 [1238]
S-Pdata1 [1238]
CPS Z-score [1238]
Criteria2 [1238]
Positive [1238]
Comment [1238]
Screenresult
Assay Well Control Type
Confirmed Positive
Excluded
Assay Well Positive
Library Well Type
Plate
Resource URI
Screen ID
Screen Title
Library
Vendor Reagent ID
Reagent Vendor
Well ID
Well
Smallmoleculeagent
ChEMBL IDs
Compound Name(s)
InChI
Restricted
Molecular Formula
Molecular Mass
Molecular Weight
PubChem CIDs
SMILES
Structure Image
Well
Deprecation Reason
Facility ID
Deprecated
Library Full Name
Library
Concentration (mg/ml)
Molar Concentration
Screen Type

Selected Columns
Unselect

Screenresult-1238
Fluorescence Polarization\_A [1238]
PChannel\_A [1238]
SChannel\_A [1238]
Fluorescence Polarization\_B [1238]
PChannel\_B [1238]
SChannel\_B [1238]
Z-score\_A [1238]
Z-score\_B [1238]
Z-score\_Avg [1238]
Criteria1 [1238]
S-Pdata1 [1238]
CPS Z-score [1238]
Criteria2 [1238]
Positive [1238]
Comment [1238]
Screenresult
Assay Well Control Type
Library Well Type
Plate
Library
Vendor Reagent ID
Reagent Vendor
Well
Smallmoleculeagent
Compound Name(s)

Cancel and return to page
Continue



It is also informative to include information from Studies, e.g. 'Reagent counts for small molecule screens' and 'Vendor-provided compound description/activity/target'. Similar to adding columns, click **Add study columns**, check all to included, then select **Continue**.

Select study columns to display

---

Available Columns

Search...

- 100001 - Annotations on Suitability of Compounds: Miscellaneous Sources
  - Unsuitable [100001]
  - Notes on Suitability [100001]
- 100002 - Annotations on Suitability of Compounds: G. Cuny & K. Lee
  - Notes on Suitability [100002]
- 100004 - Compounds found to be fluorescent at specific excitation/emission wavelengths (PubChem data)
  - Plate [100004]
  - Well [100004]
  - Pubchem CID [100004]
  - Activity [100004]
  - Excitation/Emission Wavelengths Tested [100004]
  - Pubchem Assay ID (Wavelengths Tested) [100004]
- 100005 - Compounds found to be NOT fluorescent at specific excitation/emission wavelengths (PubChem data)
  - Plate [100005]
  - Well [100005]
  - Pubchem CID [100005]
  - Activity [100005]
  - Excitation/Emission Wavelengths Tested [100005]
  - Pubchem Assay ID (Wavelengths Tested) [100005]
- 100006 - ICCB-L/NSRB compounds found to be fluorescent at the specific excitation/emission wavelengths
  - Pubchem CID [100006]
  - Activity [100006]
  - Excitation/Emission Wavelengths Tested [100006]
  - ICCB-L/NSRB Screen # [100006]
- 100007 - ICCB-L/NSRB compounds found to be cytotoxic to HIV-infected HeLa-derived TZN-bl cells at 2 uM and 10 uM.
- 100010 - Vendor-provided compound description/activity/target
- 100011 - ICCB-Longwood Mechanism of Action Library compound tool scores and protein target
- 100012 - CLUE Drug Repurposing Hub mechanism of action and target annotations
- 200001 - Reagent Counts for Small Molecule Screens
  - Positives Count [200001]
  - Screened Count [200001]
  - Positives Count (Biochemical) [200001]
  - Screened Count (Biochemical) [200001]
  - Positives Count (Cell-based) [200001]
  - Screened Count (Cell-based) [200001]
  - Positives Count (Multi-cellular organism) [200001]

Selected Columns

Depending on your data sharing level, you will have permission to view a selection of other screens conducted at ICCB-L, enabling result comparisons. To do this, you can check the button next to **Mutual positives** on the upper right side of the screen. This will add the results columns of *all screens* you have permission to view. Alternatively, if you prefer to view *specific screens or data columns* that you have permission to view, click the **Add other screen columns** and select desired columns to add.

Screen Details
Screening Summary
Protocol
Chem
Picks
Activities
Data

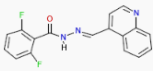
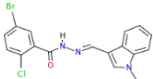
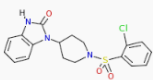
Screen Results
Data Columns

☒ Show positive rows only
☒ Mutual positives

Page 1 of 13 pages, 309 Screen Results

Rows
25

Plate	Well	Library	Structure Image	Library Well Type	Vendor Reagent ID	Compound Name(s)	Assay Well Control Type	Positive [150]	Positive-2 [150]	Abnormal Morphology [151]	Anti-Mitotic [151]	Toxic [151]	Positives [267]	Positive [299]	Positive [367]	Positive_attachment [415]	Positive_growth promoted [415]	Positive_attachment promoted [415]	Positive_S/M/W [459]	Positive_Y/N [459]	Positive_539 and 459 [459]	Positive [469]
531	M04	CEREP		Experimental	S0002577-S0000122			NP	True			null	null	null	null				null	null		
533	N12	CEREP		Experimental	S0002866-S0000187			NP	True			null	null	null	null				null	null		
534	F22	CEREP		Experimental	S0002513-S0081691			NP	True			null	null	null	null				null	null		
534	N05	CEREP		Experimental	S0004002-S0081704			NP	True			null	null	null	null				null	null		
539	C06	CEREP		Experimental	S0002986-S0000274			NP	True			null	null	null	null				null	null		
539	P05	CEREP		Experimental	S0002862-S0069903			NP	True			null	null	null	null				null	null		

Screen Details   Screening Summary   Protocol   Cherry Picks   Activities <b>Data</b>														
Screen Results <b>Data Columns</b>														
Clear searches   Select columns   Add other screen columns   Add study columns <input checked="" type="checkbox"/> Show positive rows only <input type="checkbox"/> Mutual positives <b>Download</b>														
Page 1 of 13 pages, 309 Screen Results   Rows 25														
Plate	Well	Library	Structure Image	Library Well Type	Reagent Vendor	Vendor Reagent ID	Compound Name(s)	Assay Well Control Type	Fluorescence Polarization (mP)_A [150]	mP z-score [150]	Positive-2 [150]	Notes on Suitability [100001]	Activity [100004]	Activity [100005]
531	M04	CEREP		Experimental	CEREP	S0002577.S0000122			88.5		true			
533	N12	CEREP		Experimental	CEREP	S0002866.S0000187			87.8		true			
534	F22	CEREP		Experimental	CEREP	S0002513-S0081691			86.7		true			

#### Example 4. View compound name and structure for a particular plate and well location (or multiple wells).

The most straightforward way to view particular well(s) information in Screensaver is to use the Find Plate Wells... text search option in the search bar.

Screensaver

Libraries  
Screens  
My Screens  
Studies  
Cherry Pick Requests  
Activities  
Reports

Find a User...  
Find a Screen...  
Find a Library...

Find  
Plate Wells...  
Compound Name or Vendor ID...  
Plate & Copy...

The text search allows for different syntaxes when searching plate and well. For example, to search for plate 2089 well D05, you can enter 2089 D05, 2089:D05, or 2089D05. Clicking on ? to the right of Find will display a list of acceptable search combinations.

Compound information is displayed under 3 tabs:

**Well Details:** Provides information about the compound, including structure, vendor ID and SMILES string

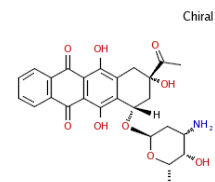


**Annotations:** Provides information on all studies pertaining to the particular compound

**Other Wells With Reagent:** If the compound is present in multiple well locations, it will be displayed in this tab. Determination is based on vendor name and ID. The same compound from different vendors will not be displayed in this tab.

Well 02089:D05

Well Details	Annotations	Other Wells With Reagent
<div>historydownload</div>		
Plate:	2089	
Well:	D05	
Library:	Biomol4	
Facility ID:	ICCB-802277	
Library Full Name:	Biomol 4 - FDA Approved Drug Library	
Screen Type:	Small Molecule	
Concentration (mg/ml):	2	
Library Well Type:	Experimental	
Is Deprecated:	False	
Vendor:	BIOMOL	
Vendor Reagent ID:	DL-548	
SMILES:	<chem>c([C@@@]([H])(O)[C@@@H]1O[C@@@H](C)[C@@@H](O)[C@@@H](N)C1)C[C@](O)(C(=O)C)C2)(c(O)c(c3c4O)C(=O)c(c5C3=O)cccc5)c24</chem>	
InChI:	InChI=1S/C26H27NO9/c1-10-21(29)15(27)7-17(35-10)36-16-9-26(34,11(2)28)8-14-18(16)25(33)20-19(24(14)32)22(30)12-5-3-4-6-13(12)23(20)31/h3-6,10,15-17,21,29,32-34H,7-9,27H2,1-2H3/t10-,15-,16-,17-,21+,26-	
Molecular Formula:	C26H27NO9	
Molecular Mass:	497.17	
Molecular Weight:	497.49	
Compound Names:	Idarubicin	
PubChem CIDs:	42890	
ChemBank Ids:		
ChEMBL Ids:		
Other Wells With Reagent:	02055:D05, 02073:D05	
Is Restricted:	False	



The above examples illustrate how to access some of the information within Screensaver. We encourage you to look around on your own, building on what is described here. Please contact the ICCB-L team with any questions you have, issues encountered or feedback you would like to provide.