Screensaver User Manual

Screensaver is an open source, web based *L*aboratory *I*nformation *M*anagement *S*ystem (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.

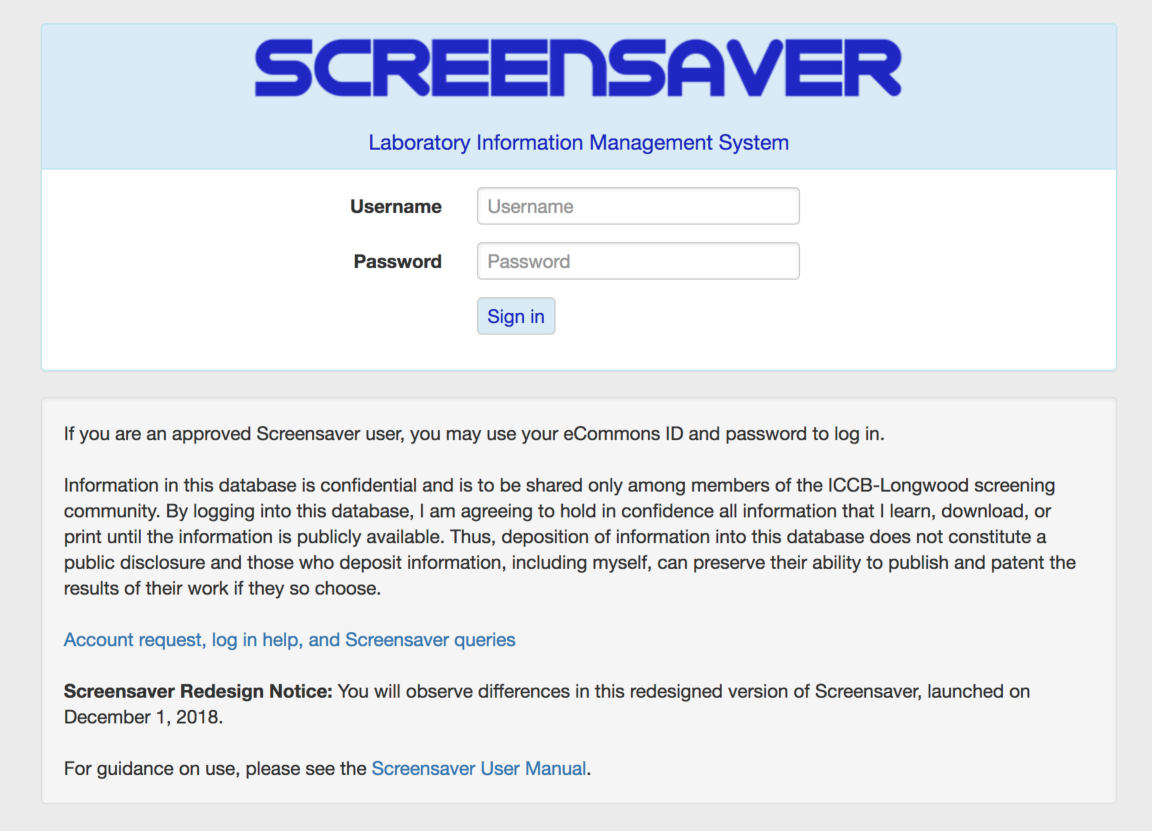
Example 2 (page 5): Identify which small molecule libraries contain compounds that target EGFR.

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

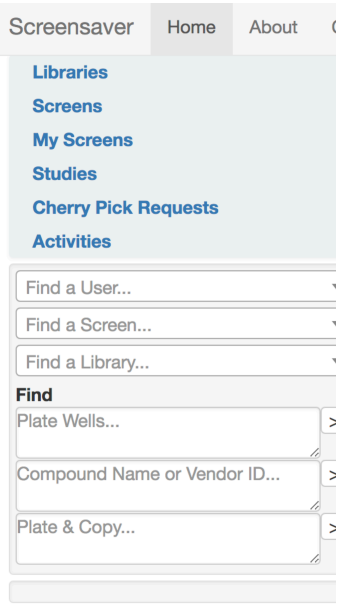
Example 4 (page 10): View compound name and structure for a particular plate and well location (or multiple wells).

Getting started:

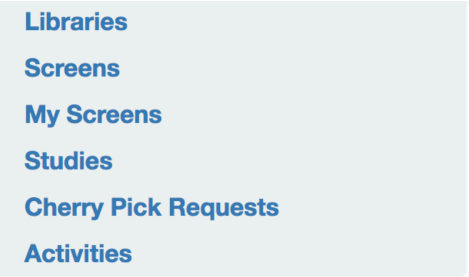
To sign in, go to the Screensaver sign page (https://screensaver.med.harvard.edu) and enter your eCommons ID and password, then click **Sign in**.



The 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.



Menu Navigation



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.

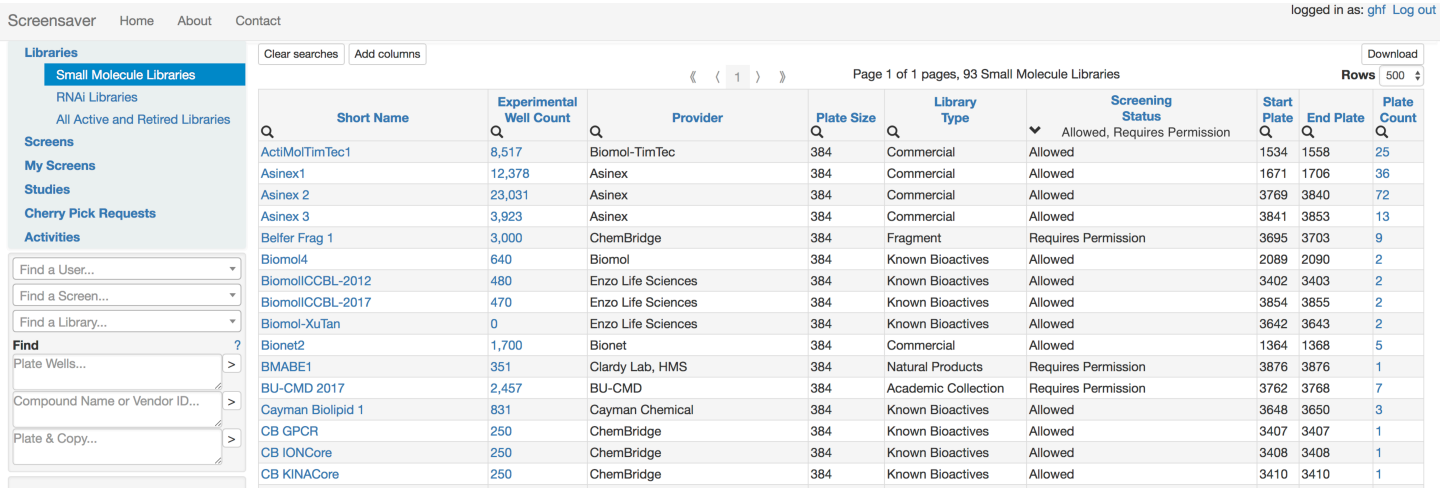
Cherry Pick Requests: A list of User's cherry pick requests.

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.

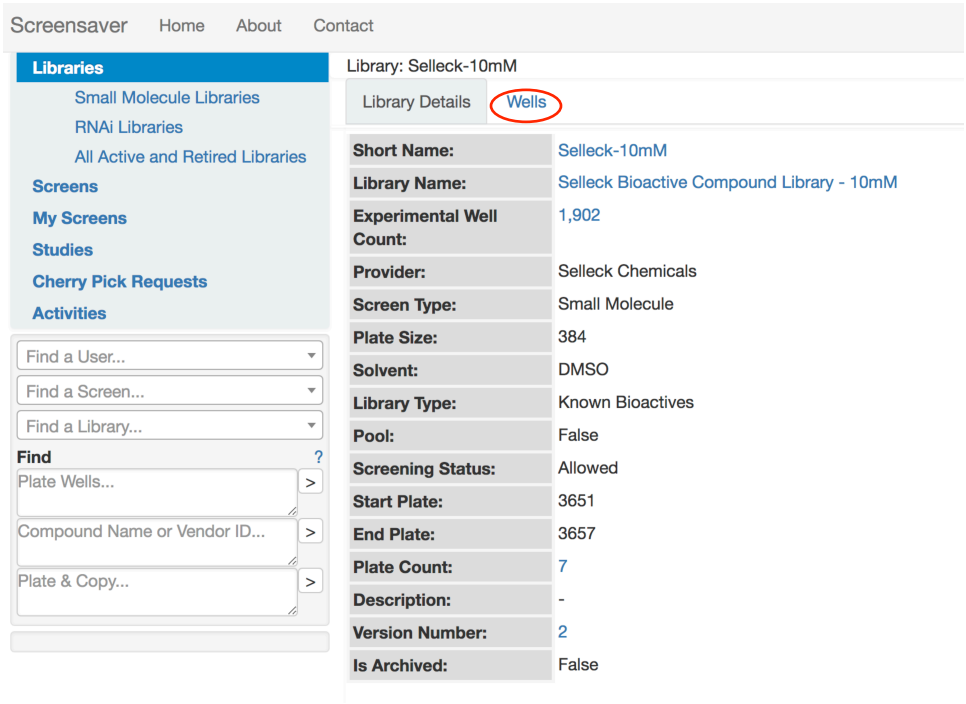
Select **Libraries**, then **Small Molecule Libraries**. Libraries appear alphabetically and you can scroll to the one of interest.



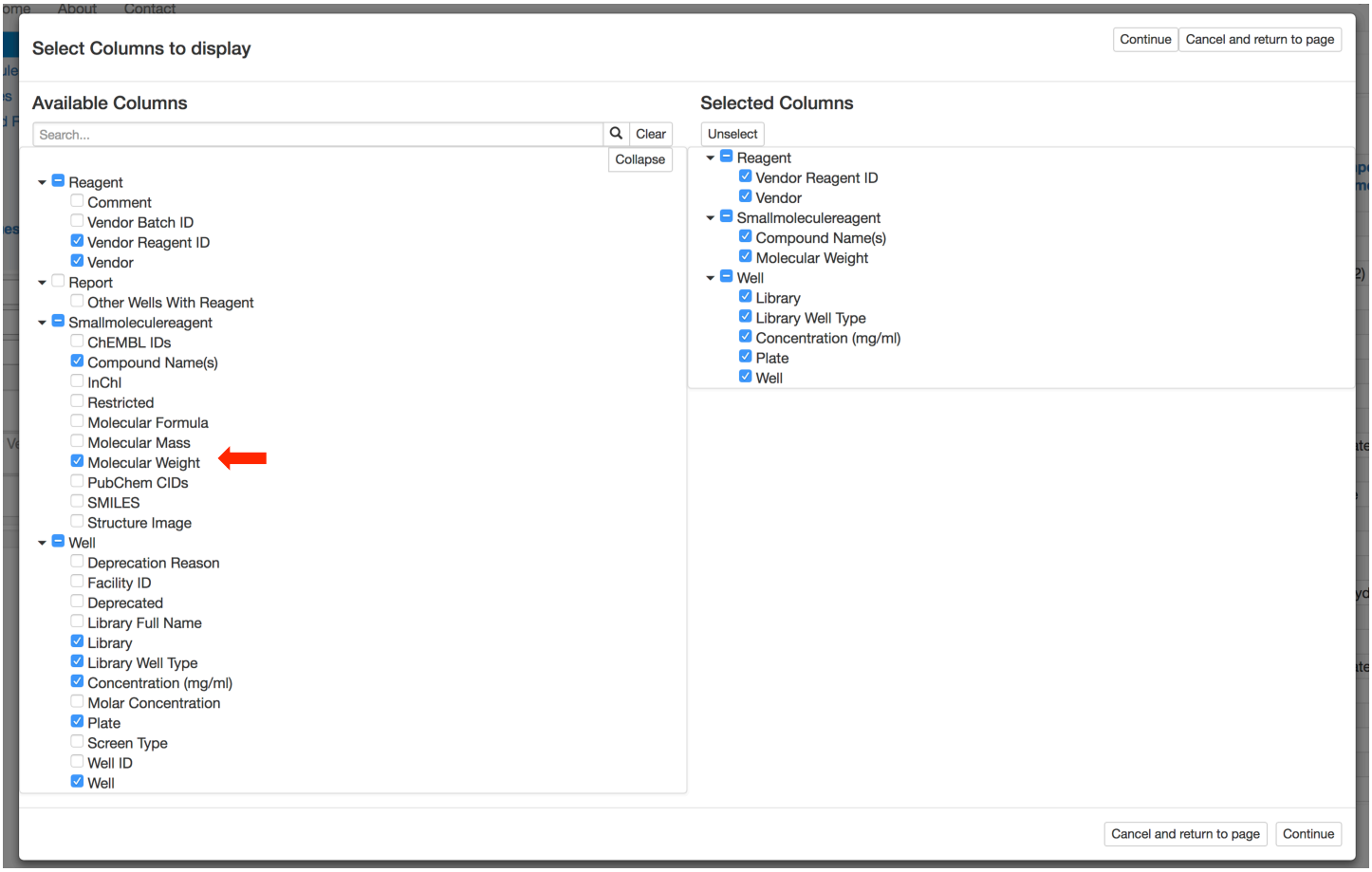
Short Name	Experimental Well Count	Provider	Plate Size	Library Type	Screening Status (Allowed, Requires Permission)	Start Plate	End Plate	Plate Count
ActiMolTimTec1	8,517	Biomol-TimTec	384	Commercial	Allowed	1534	1558	25
Asinex1	12,378	Asinex	384	Commercial	Allowed	1671	1706	36
Asinex 2	23,031	Asinex	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.



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.



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

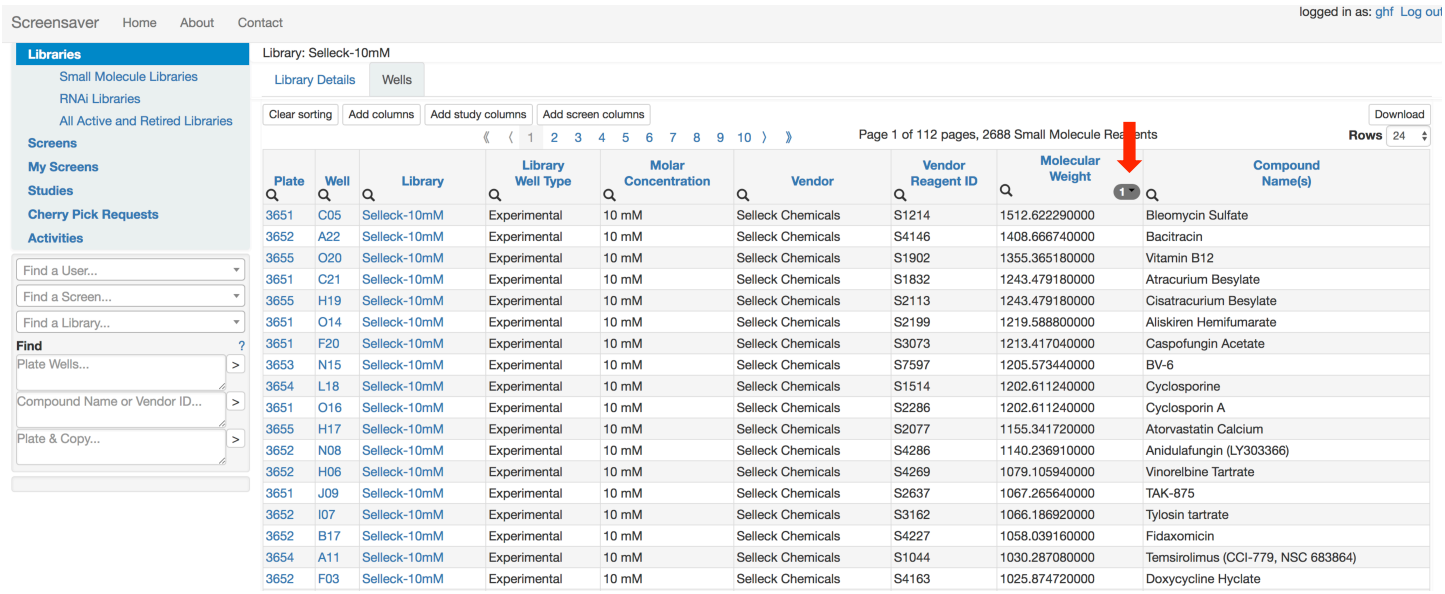
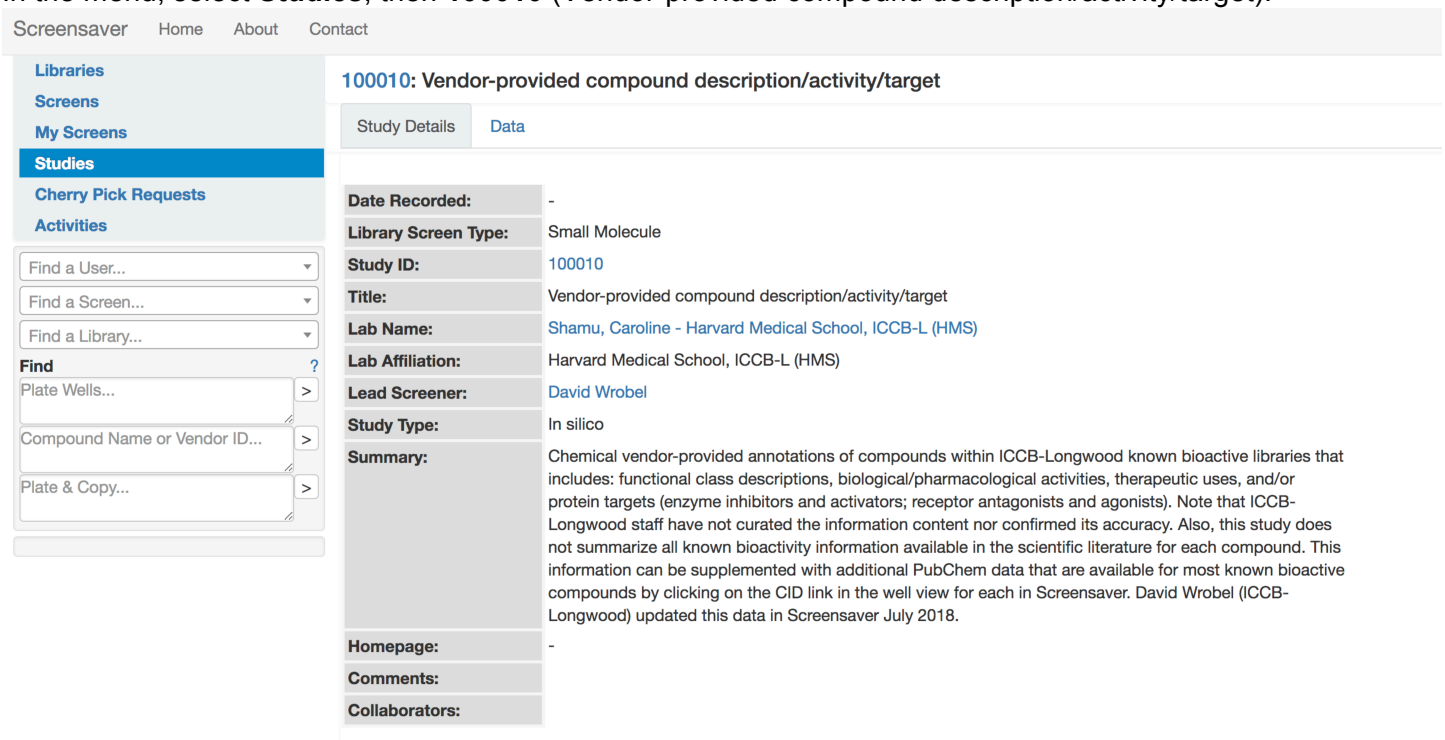


Plate	Well	Library	Library Well Type	Molar Concentration	Vendor	Vendor Reagent ID	Molecular Weight	Compound Name(s)
3651	C05	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S1214	1512.622290000	Bleomycin Sulfate
3652	A22	Selleck-10mM	Experimental	10 mM	Selleck Chemicals	S4146	1408.666740000	Bacitracin
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

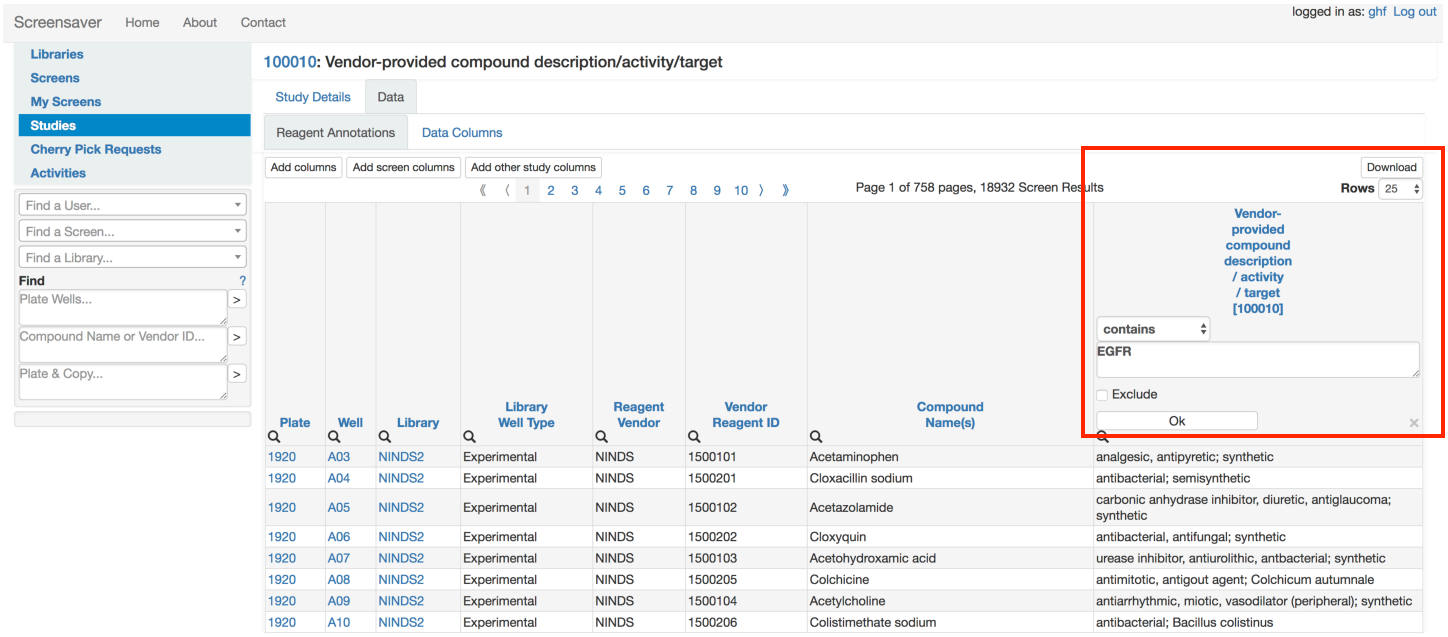
If you wish to view or manipulate the data in another program (eg Excel, Vortex, KNIME), click **Download** to export the data. Prior to downloading, confirm all desired columns are visible. Only columns displayed in the table will be downloaded. Available formats for export are xlsx, csv and sdf.

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

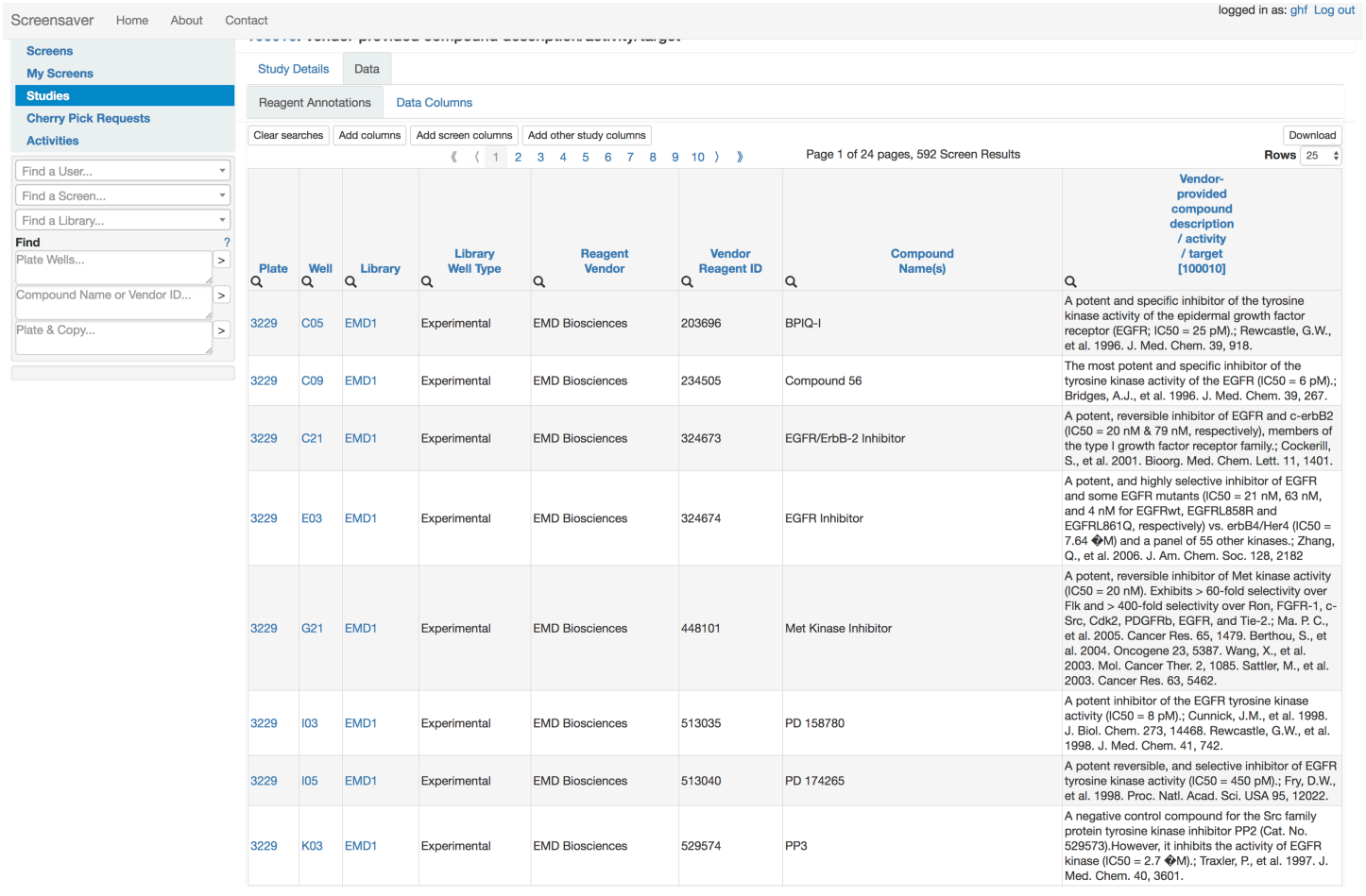
In the menu, select **Studies**, then **100010** (Vendor-provided compound description/activity/target).



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**.

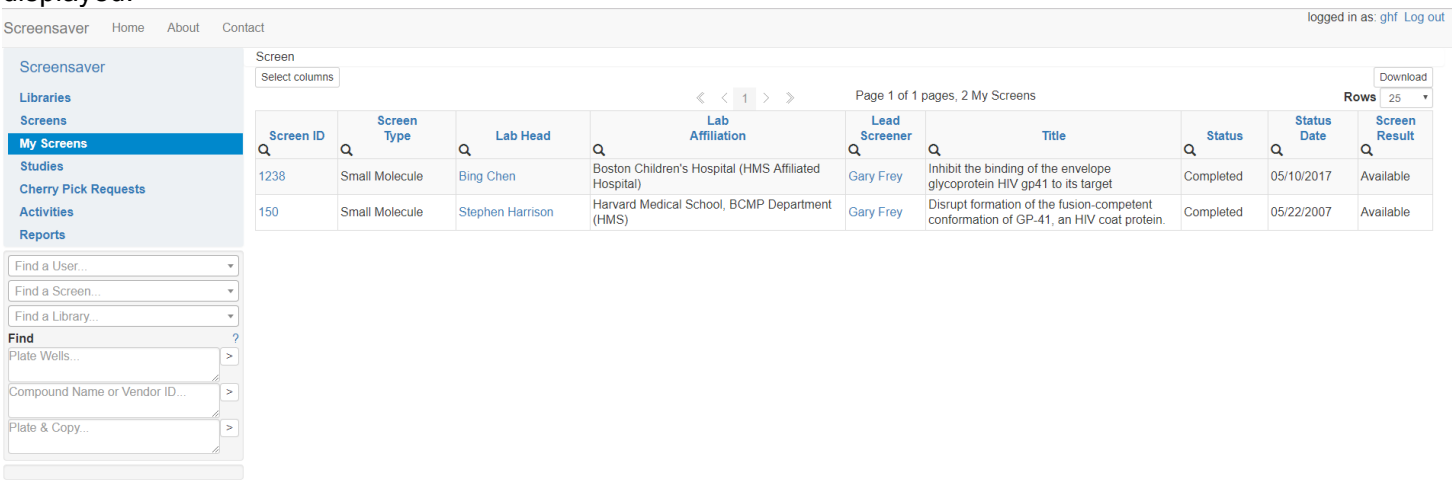


The updated table will contain a list of all experimental wells in which the vendor has indicated EGFR as a target.

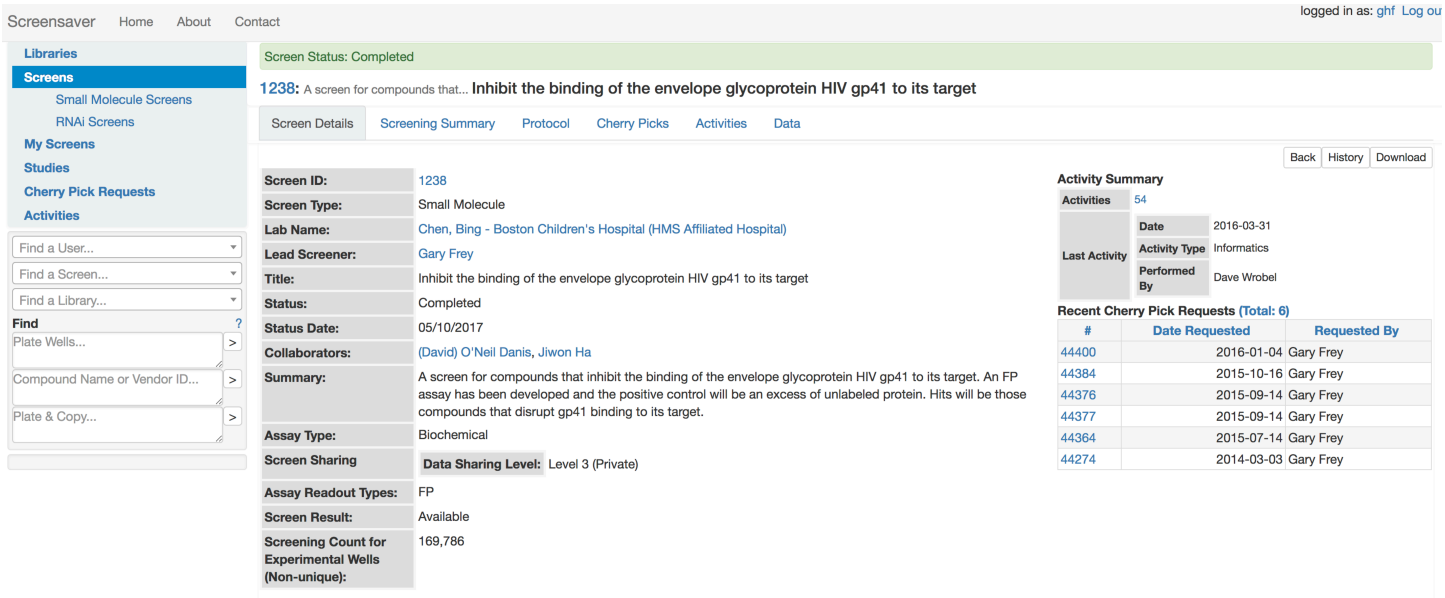


Example 3. Download a file of all potential hits identified in User's screen, including columns for compound structure and compound ID.

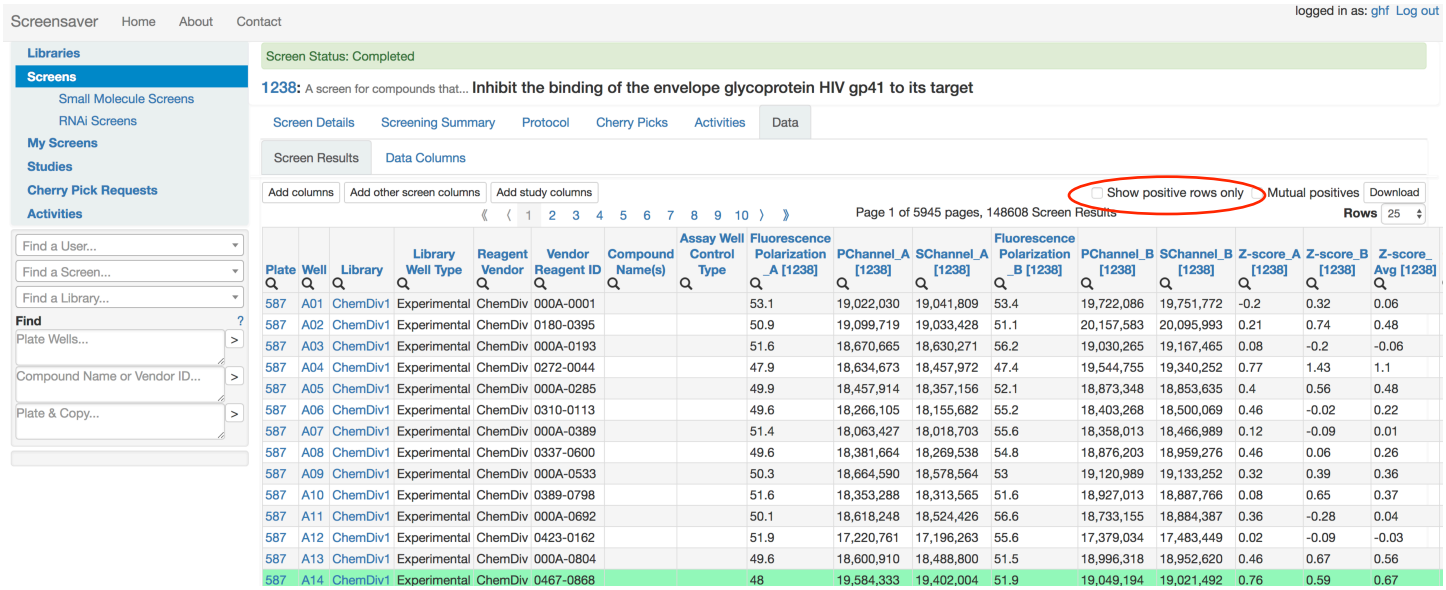
In the search menu, select **My Screens**. A list of all screens you conducted or collaborated on at ICCB-L are displayed.



Click **Screen ID #** of interest.

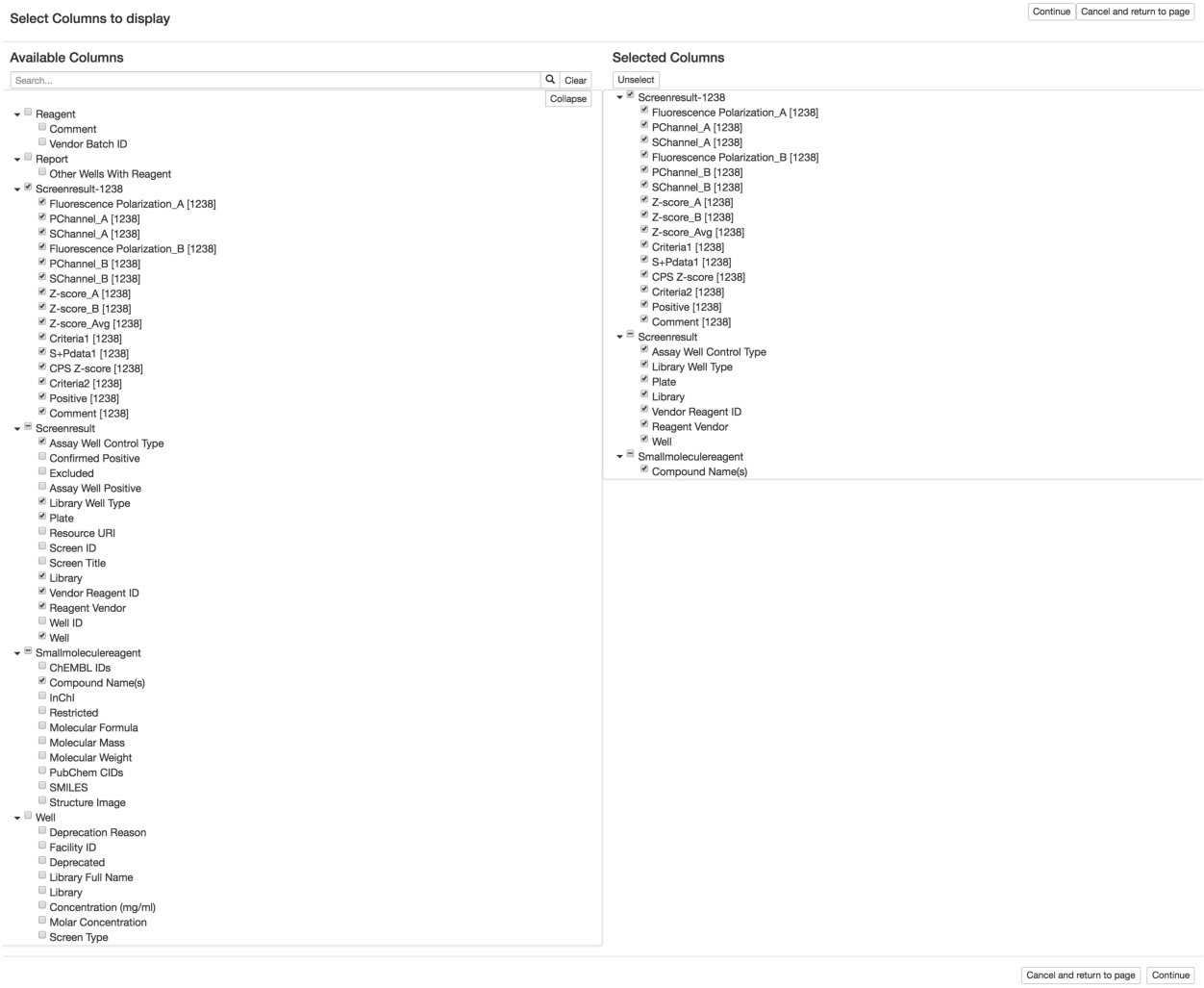


The **Screening Summary** tab provides more detailed information, including the option to view all **Plates Screened** and **Libraries Screened**. The protocol provided in the primary screen report can be viewed by clicking **Protocol**. Any cherry picks requests and the corresponding plate maps can 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**.

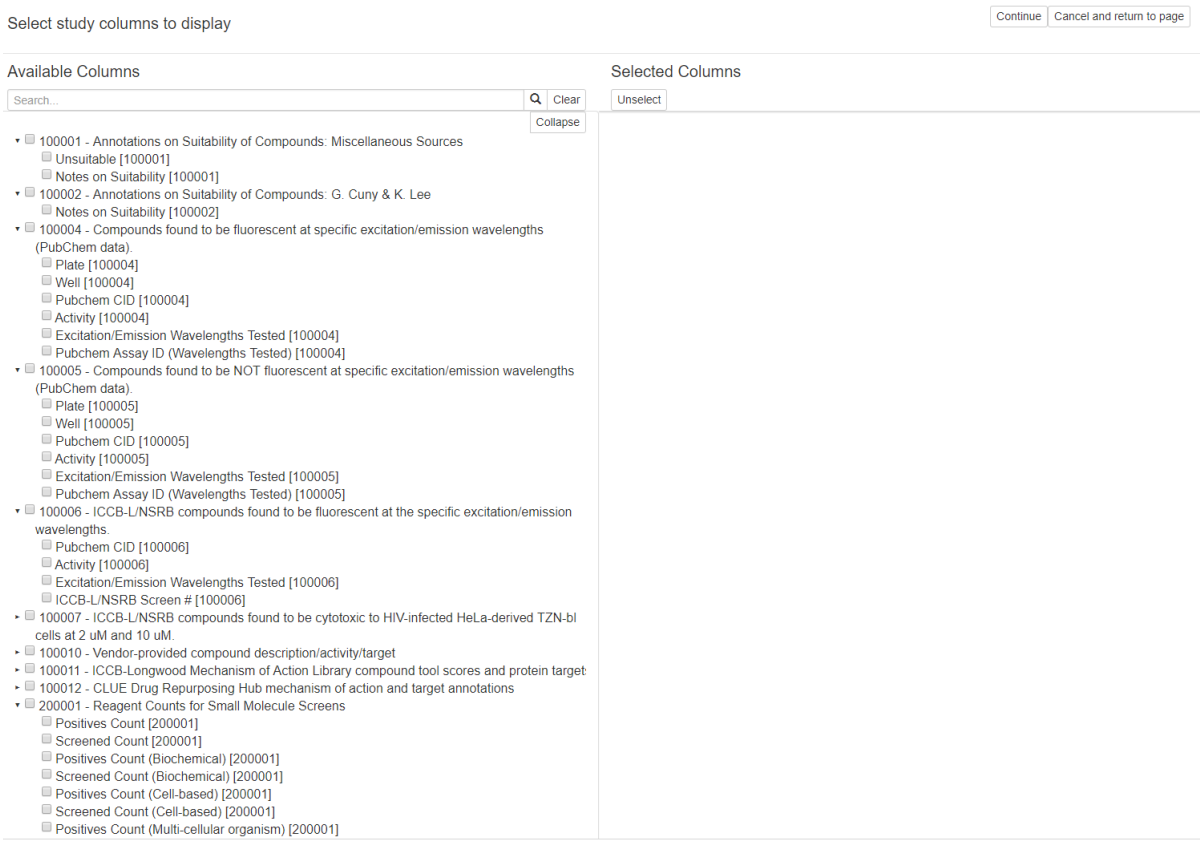


All results are displayed. Depending upon the number of data columns, the table may continue out of view to the right. To only display potential hits, select the box next to **Show positive rows only.**

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**.



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**.



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.

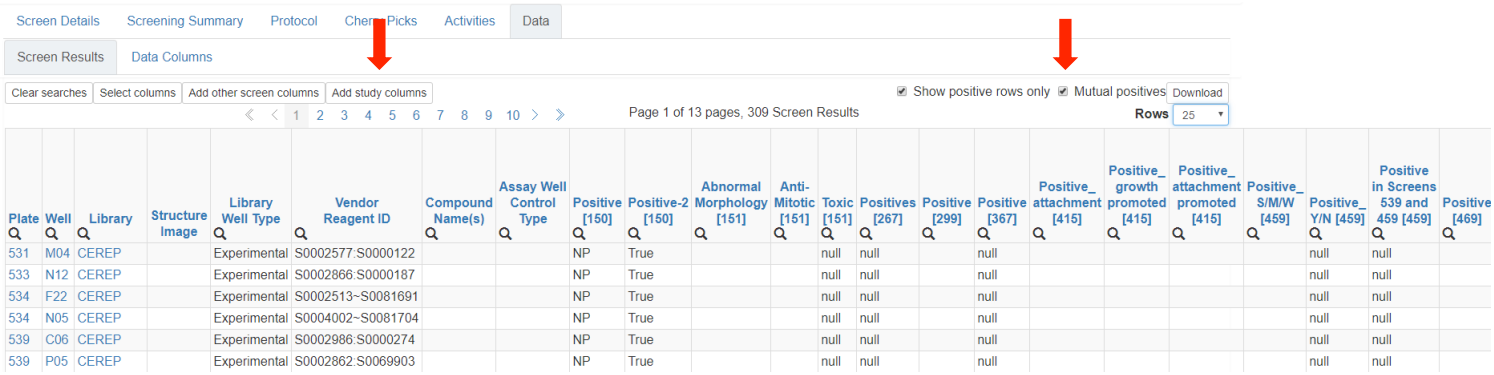


Plate	Well	Library	Structure Image	Library Well Type	Vendor Reagent ID	Compound Name(s)	Assay Well Control Type	Positive [150]	Positive-2 [150]	Abnormal Morphology [151]	Anti-Mitotic [151]	Toxic [151]	Positives [267]	Positive [299]	Positive [367]	Positive_ attachment [415]	Positive_ growth promoted [415]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

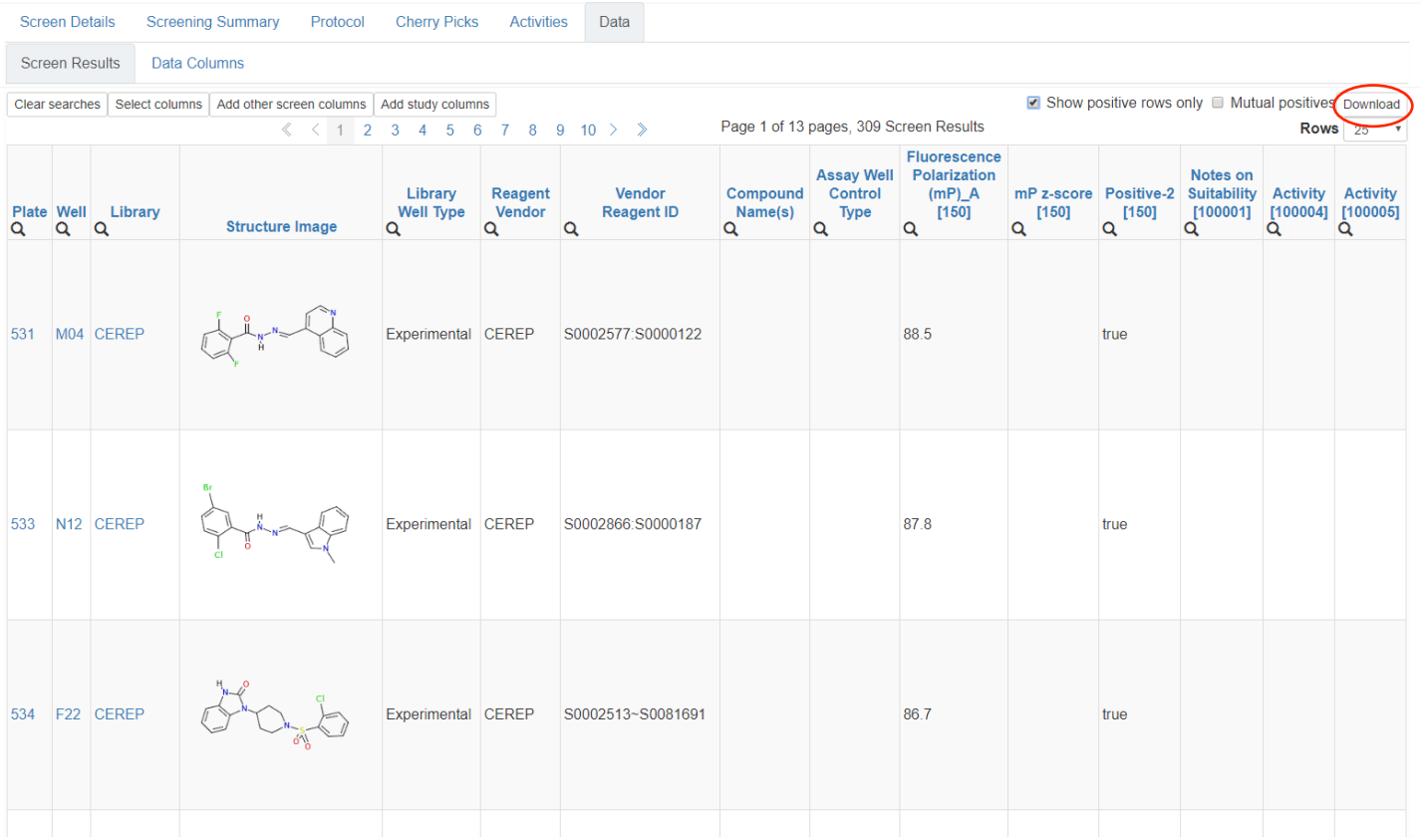
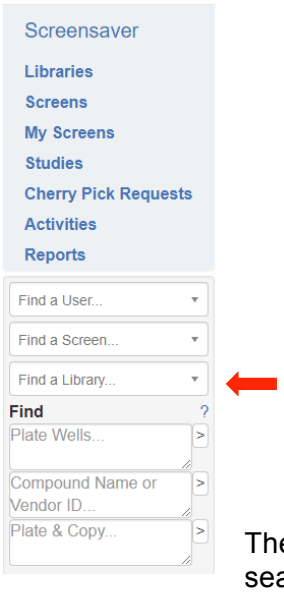


Plate	Well	Library	Structure Image	Library Well Type	Reagent Vendor	Vendor Reagent ID	Compound Name(s)	Assay Well Control Type	Fluorescence Polarization (mP)_A [150]	mP z-score [150]	Positive-2 [150]	Notes on Suitability [100001]	Activity [100004]	Activity [100005]
531	M04	CEREP		Experimental	CEREP	S0002577:S0000122			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.



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.

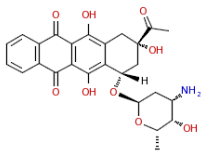
Well 02089:D05

Well Details | Annotations | Other Wells With Reagent

history | download

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:	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
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

Chiral



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.