

## Overview: ICCB-L Screening Facility User Agreement for Small Molecule Screening Projects

There are two different ICCB-L User Agreements, one for small molecule screeners and one for RNAi screeners. Small molecule user agreements apply only to small molecule screening projects and data; RNAi agreements apply only to RNAi projects and data. Screeners carrying out both small molecule and RNAi screening projects at ICCB-L must sign both small molecule and RNAi user agreements. All Users from the same research group must choose the same data sharing level, with the decision to be made by the principal investigator of that group.

The right of users to perform screens at ICCB-L is solely at the discretion of the ICCB-L Directors and the ICCB-L scientific advisory committee. By signing the agreement, all users agree to deposit annotated screening data into Screensaver, to hold in confidence all unpublished data that they access about other screens via Screensaver, and to allow ICCB-L to use their data for quality control improvements and statistical analysis.

This agreement requires each small molecule screener to choose a level of pre-publication data sharing: Level 1, Level 2, or Level 3. The main points regarding each level are summarized below. Although sharing small molecule screening data prior to publication is not required of ICCB-L screeners, we strongly recommend it and encourage you to share your data at Level 1 or Level 2. In our experience, the benefits of sharing small molecule primary screen results before publication within the community of ICCB-L screeners far outweigh any potential risks. We believe that the new ICCB-L policies are fair and will meet the requirements of NIH data sharing guidelines. Further, we have been advised that sharing data within the context of Screensaver does not constitute public disclosure for patent purposes. However, individuals may wish to consult with their own patent counsel as appropriate.

Regardless of the level of participation chosen by a screener, all annotated small molecule screening data must be deposited into Screensaver in a timely manner, as it is obtained. Upon publication, data from screens conducted at ICCB-L will be made available to all Screensaver users. The data sharing agreement (and access to Screensaver) will expire two years from the date of execution. However, screeners who wish to retain access to Screensaver may renew their data sharing agreement. Screening data will be shared at Level 1 and 2 beginning two years after completion of each screen, as defined jointly by each screen's principal investigator and ICCB-L staff. We will also work with screeners to format post-publication data for entry into the PubChem database (<http://pubchem.ncbi.nlm.nih.gov/>), which is publicly available.

### Pre-publication sharing options for small molecule screen data:

**Level 3:** Screening data are not shared with other Screensaver users, unless they are designated as collaborators by the lead screener or PI of the screen. Screeners automatically become Level 3 users when their projects are accepted for piloting or screening at ICCB-L. Level 3 Users have access only to basic information about ICCB-L compound and RNAi libraries, information about their own screening project(s), and data from published screens.

**Level 2:** Only data related to Overlapping Hits are shared among Level 2 users. Level 2 users will also have access to Overlapping Hit information from Level 1 screens. An Overlapping Hit is defined as a compound that has been annotated as a positive in another screen. Data that will be shared for each Overlapping Hit include:

- titles and brief general descriptions of other screens that also scored the compound as a positive

- identity and contact information for investigator(s) associated with screens that have Overlapping Hits
- summary experimental and data analysis protocols for screens that have Overlapping Hits
- whether the Overlapping Hit was chosen as a cherry pick, and whether the cherry pick was confirmed as a positive in those screens

**Level 1:** All data are shared among Level 1 users. Level 1 users will also have access to Overlapping Hit information from Level 2 screens.

Signed forms should be sent to Dr. Jennifer Smith at the address below. Electronic copies are preferred if possible.

Jennifer A. Smith, Ph.D.  
Seeley Mudd 604, Harvard Medical School  
250 Longwood Avenue  
Boston, MA 02115 USA  
jennifer\_smith@hms.harvard.edu  
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# ICCB-Longwood Screening Facility User Agreement

## Small Molecule Screening Projects

This User Agreement will govern the use by \_\_\_\_\_ *[insert name of investigator]* (“You” or “User”) of the ICCB-Longwood Screening Facility and Your access to screening data generated at the facility by other users. More information about ICCB-Longwood (ICCB-L) can be found at <http://iccb.med.harvard.edu>.

ICCB-L is a screening facility that serves a community of scientists. The data that each user generates in his or her screening project(s) at ICCB-L may be useful to other users, and ICCB-L and the NIH support the broad sharing of such data to benefit the overall scientific community and to accelerate scientific discovery. This User Agreement creates a mechanism for You to have access to information deposited by other ICCB-L users into the internal, non-public ICCB-L database (called “Screensaver” and further described on the ICCB-Longwood website), and for other users to have access to the information that You deposit, at the applicable data access/sharing level described below. Along with executing this User Agreement, You must choose one of the data access/sharing levels indicated below by initialing in the corresponding place.

### 1. General

**1.1.** You acknowledge that the information You deposit into Screensaver may be used by ICCB-L for quality control improvements and statistical analysis (e.g., how often a specific compound has been identified as a positive, and whether it displays undesirable properties). You agree that such statistical analysis may be made public at any time by ICCB-L, provided that the details of Your screening approach and the specific structures of Your hits are not released other than as permitted under the data access/sharing level You choose above. ICCB-L will do its best to inform You when information abstracted from Your screen(s) is made public.

**1.2.** You agree to hold in confidence all data to which You gain access under this User Agreement until, and then only to the extent that, such data are publicly available or You have obtained express written consent to publish or otherwise publicly disclose such data from the user who deposited such data. The purpose of this requirement is to avoid having the deposition of data into Screensaver constitute a public disclosure so that those who deposit data, including You, can preserve their ability to patent the results of their work if they so choose. You understand that You may discuss such data with members of Your laboratory, but only if You first require them to sign a confidentiality agreement that prohibits them from sharing such data with others until they are publicly available. If You do obtain express written consent to publish or publicly disclose another user’s unpublished data, You will acknowledge such user appropriately. In addition, You will notify the ICCB-L Directors if work You performed in the ICCB-L facility results in a publication, and You will formally acknowledge the contribution made by ICCB-L and, if appropriate, specific ICCB-L personnel.

**1.3.** You agree to acknowledge the support of the ICCB-L in publications arising from your use of the facility. If an ICCB-L member has made an important intellectual contribution to the project, as determined by generally accepted criteria for academic collaborations, then that person should be considered for authorship on the publication. **For projects supported by the NERCE or the NSRB, you must cite award number U54 AI057159 from the National Institute of**

**Allergy and Infectious Diseases (NIAID) and fulfill all NIH stipulations regarding citation of support in publications.** If your project was supported by a grant that also directly supports the ICCB-L, please consult the ICCB-L Director regarding the appropriate grant citation.

**1.4.** Your right to perform screens at ICCB-L is solely at the discretion of the ICCB-L Directors and the ICCB-L scientific advisory committee. The Directors will have the right to limit Your access to ICCB-L facilities and technical support to that which is required to perform scope of work contained in Your proposal(s) and approved by the Directors and the scientific advisory committees. In the event of a disagreement as to the scope and/or duration of such work, You may discuss the matter with the Directors and the scientific advisory committees, who then will make a binding decision as to the extent of Your permitted use of ICCB-L facilities.

**1.5.** You acknowledge that You are aware the ICCB-Longwood screening fees and associated F&A are revised annually based upon the Harvard Fiscal Year (July 1 – June 30). New fees are typically recalculated in August or early September and are retroactive for any screening fee milestone reached on or after July 1 of the current fiscal year. The fee structure is updated on the ICCB-Longwood website as soon as it is available. By signing below, You acknowledge all charges are based on the screening fee at the time of service, not a previously provided estimate or price structure from a previous fiscal year.

**1.6.** If You are not employed by Harvard, You represent that the institution with which you are affiliated is responsible for providing any environmental, health and laboratory safety training required by law or regulation with respect to the work that you intend to conduct at ICCB-L. This training may include, but is not limited to, laboratory safety, biosafety, chemical safety, hazard communication, spill prevention, occupational exposure to bloodborne pathogens, hazardous waste management and personal protective equipment training. By signing below, You and an authorized representative of Your institution acknowledge that You have completed all training applicable to the work that you intend to conduct at ICCB-L.

## **2. Data Access/Sharing**

By signing this User Agreement and using the ICCB-Longwood facility, You are agreeing to deposit *all* information and annotated data with respect to Your screening project(s) conducted at ICCB-L (e.g., screen title(s), screening protocol(s), criteria for defining screening positives, raw data obtained from your screen(s), lists of screening positives, lists of cherry picks, cherry pick confirmation data, lists of re-ordered compounds and results of follow-up experiments) into Screensaver in a timely manner, as such information becomes available, regardless of the data access/sharing level that You choose. For the purposes of this document, the term "annotated data" refers to screening data that have been analyzed by the screener and resubmitted to ICCB-L along with the screen experimental protocol, lists of screening positives, and a description of how compounds were defined as positives in the screen.

For projects supported by the NERCE or the NSRB, You agree that upon publication of the primary results of Your screen, all data associated with Your screening project may be made public by deposition in PubChem (<http://pubchem.ncbi.nlm.nih.gov/about.html>). For ICCB-L screeners who are not part of the NERCE/NSRB program, we encourage (but do not require) You to deposit Your published screening data into PubChem, and can work with You to facilitate the PubChem deposition process.

All Users from the same research group must choose the same data sharing level, with the decision to be made by the principal investigator of that group.

**2.1. Level 1 User**     \_\_\_[initial here if You choose to be a Level 1 User once You have deposited Your annotated small molecule screening data into Screensaver]

(a)     **Level 1 User Option.** If You choose this option, Your Level 1 User status will be activated when you begin to deposit annotated small molecule screening data into Screensaver (or immediately if You deposited annotated screening data into Screensaver under a User Agreement that expired within the 6 months prior to the date You renew your access to the ICCB-L facility by signing this User Agreement). Prior to then, you automatically will be a Level 3 User, as specified in Section 1.3 below.

(b)     **Level 1 User Data Access Rights.** A Level 1 User may access all data (including raw data and lists of positives) associated with screens conducted at ICCB-L by other Level 1 Users. In addition, a Level 1 user may access all of the information described in Section 1.2(b) from screens conducted at ICCB-L by Level 2 Users.

(c)     **Level 1 User Data Sharing Obligations.** All screening data that have been published by Level 1 Users will be made available to all ICCB-L users. In addition, all data (including raw data and lists of positives) associated with unpublished screens that a Level 1 User conducted at ICCB-L will be made available to all other Level 1 Users. Also, all of the information described in Section 1.2(b) from screens on compounds that a Level 1 User conducted at ICCB-L will be made available to all Level 2 Users who have Overlapping Hits (as defined below in Section 1.2(b)) with such compounds.

(d)     **Changing Your Level 1 User Status.** After electing to be a Level 1 User, if you wish to change your status, you must provide a written request and justification to the ICCB-L Directors and the ICCB-L scientific advisory committee, which will have sole, binding discretion in approving or denying Your request. If the scientific advisory committee decides to approve Your request, all data (including raw data and lists of positives) associated with screens that You conducted at ICCB-L while You were a Level 1 User will remain available to all other Level 1 Users.

**2.2. Level 2 User**     \_\_\_[initial here if You choose to be a Level 2 User once You have deposited Your annotated small molecule screening data into Screensaver]

(a)     **Level 2 User Option.** If You choose this option, Your Level 2 User status will be activated when you begin to deposit annotated small molecule screening data into Screensaver (or immediately if You deposited annotated screening data into Screensaver under a User Agreement that expired within the 6 months prior to the date You renew your access to the ICCB-L facility by signing this User Agreement). Prior to then, you automatically will be a Level 3 User, as specified in Section 1.3 below.

(b)     **Level 2 User Data Access Rights.** A Level 2 User may access the titles of all screens in Screensaver, the names of the associated investigators, and data associated with published screens. In addition, a Level 2 User may access the following types of information in Screensaver, but only with respect to compounds that such Level 2 User has annotated as "positive" in a screen that he or she conducted at ICCB-L ("Overlapping Hits"):

(i) whether the positive compound also scored as a positive in other screens ("Overlapping Hit"), including information on hit strength, whether the Overlapping Hit was chosen as a cherry pick, and whether the cherry pick was confirmed as a positive;

(ii) titles and brief general descriptions of screens that also scored the compound as a positive (“Hit Overlap Screens”);

(iii) identity and contact information for investigator(s) associated with Hit Overlap Screens; and

(iv) summary experimental and data analysis protocols for Hit Overlap Screens, to help with interpretation of the relevance of the overlapping hit list provided.

**(c) Level 2 User Data Sharing Obligations.** All screening data that have been published by Level 2 Users will be made available to all ICCB-L users. In addition, the titles of all screens conducted at ICCB-L by a Level 2 User, along with the fact that he or she is the associated investigator, will be made available to all other Level 2 Users and all Level 1 Users. Also, all of the information described in Section 1.2(b) from screens on compounds that a Level 2 User conducted at ICCB-L will be made available to all other Level 2 Users and all Level 1 Users who have Overlapping Hits for such compounds. Finally, all data (including raw data and lists of positives) associated with each screen that a Level 2 User conducted at ICCB-L will be made available to all Level 1 Users two years after completion of such screen, even if such screen is unpublished; provided, however, that a Level 2 User may seek a delay of such obligation by providing a written justification for such delay to the ICCB-L scientific advisory committee. The completion date of an individual screen will be determined jointly by the screen principal investigator and the ICCB-L staff.

**(d) Changing Your Level 2 User Status to Level 1 User Status.** After electing to be a Level 2 User, you may choose to change Your status to that of a Level 1 User upon written notification to the ICCB-L Directors. If you do so, the data (including raw data and lists of positives) associated with screens that You conducted at ICCB-L while You were a Level 2 User will become available to all Level 1 Users.

**(e) Changing Your Level 2 User Status to Level 3 User Status.** After electing to be a Level 2 User, if you wish to change your status to that of a Level 3 User, you must provide a written request and justification to the ICCB-L Directors and the ICCB-L scientific advisory committee, which will have sole, binding discretion in approving or denying Your request. If the advisory committee decides to approve Your request, all data (including raw data and lists of positives) associated with screens that You conducted at ICCB-L while You were a Level 2 User will remain available to all other Level 2 Users as specified in this Section 1.2.

**2.3. Level 3 User**        *[initial here if You choose to remain a Level 3 User after You have deposited Your annotated small molecule screening data into Screensaver]*

**(a) Level 3 User Option.** You will automatically become a Level 3 User when you initiate a screening project at ICCB-L. If You initial above, You will remain a Level 3 User after You have deposited annotated small molecule screening data into Screensaver. This data access/sharing level is appropriate to choose if You do not wish to share Your non-published screen-specific information with other ICCB-L users.

**(b) Level 3 User Data Access Rights.** A Level 3 User may access only the following types of information in Screensaver: (i) names, structure information, molecular masses and formulas, and PubChem and ChemBank IDs for small molecule reagents; (ii) gene names, EntrezGene IDs and symbols, GenBank accession numbers, and species name for RNA

silencing reagents; (iii) vendor information; and (iv) data associated with published small molecule screens.

(c) **Level 3 User Data Sharing Obligations.** All screening data that have been published by Level 3 Users will be made available to all ICCB-L users. In addition, all data (including raw data and lists of positives) associated with each screen that a Level 3 User conducted at ICCB-L will be made available to all Level 1 Users two years after completion of such screen, even if such screen is unpublished; provided, however, that a Level 3 User may seek a delay of such obligation by providing a written request and justification for such delay to the ICCB-L scientific advisory committee, which will have sole, binding discretion in approving or denying such request. Similarly, two years after completion of a screen, Overlapping Hit data (as defined above in Section 1.2(b)) associated with each screen that a Level 3 User conducted will be made available to all Level 2 Users who have Overlapping Hits with those compounds. The completion date of an individual screen will be determined jointly by the screen principal investigator and the ICCB-L staff.

(d) **Changing Your Level 3 User Status to Level 1 or Level 2 User Status.** After electing to be a Level 3 User, you may choose to change Your status to that of a Level 1 or Level 2 User upon written notification to the ICCB-L Directors. If you do so, the data (including raw data and lists of positives) associated with screens that You conducted at ICCB-L while You were a Level 3 User will become available to all Level 1 Users and/or Level 2 Users, as applicable, as specified above.

### **3. Additional points**

**3.1.** ICCB-L PROCEDURES, METHODS, DATABASES AND TOOLS ARE LIMITED IN PURPOSE AND ARE EXPERIMENTAL. HARVARD EXPRESSLY DISCLAIMS ANY AND ALL IMPLIED OR EXPRESS WARRANTIES AND MAKES NO EXPRESS OR IMPLIED WARRANTIES OF MERCHANTABILITY OR FITNESS FOR ANY PARTICULAR PURPOSE OF SUCH PROCEDURES, METHODS, DATABASES AND TOOLS OR ANY ASSISTANCE, EQUIPMENT OR INFORMATION SUPPLIED BY HARVARD, ICCB-L OR THEIR EMPLOYEES.

**3.2.** You shall be responsible for Your own acts in Your use of ICCB-L facilities, including Your performance of screens at ICCB-L, and Your use of Your screening results and data generated at ICCB-L by other users to which you gain access under this User Agreement. IN NO EVENT SHALL HARVARD, ICCB-L OR THEIR EMPLOYEES BE LIABLE FOR ANY INDIRECT, SPECIAL, PUNITIVE, INCIDENTAL OR CONSEQUENTIAL DAMAGES (INCLUDING, WITHOUT LIMITATION, DAMAGES FOR LOSS OF PROFITS OR EXPECTED SAVINGS OR OTHER ECONOMIC LOSSES, OR FOR INJURY TO PERSONS OR PROPERTY) ARISING OUT OF OR IN CONNECTION WITH THIS AGREEMENT OR ITS SUBJECT MATTER, REGARDLESS OF WHETHER HARVARD OR ICCB-L KNOWS OR SHOULD KNOW OF THE POSSIBILITY OF SUCH DAMAGES. THE AGGREGATE LIABILITY OF HARVARD, ICCB-L AND THEIR EMPLOYEES FOR ALL DAMAGES OF ANY KIND RELATING TO THIS AGREEMENT OR ITS SUBJECT MATTER SHALL NOT EXCEED THE AMOUNT PAID BY YOU OR THE INSTITUTION(S) WITH WHICH YOU ARE AFFILIATED TO HARVARD UNDER THIS AGREEMENT. THE FOREGOING EXCLUSIONS AND LIMITATIONS SHALL APPLY TO ALL CLAIMS AND ACTIONS OF ANY KIND, WHETHER BASED ON CONTRACT, TORT (INCLUDING BUT NOT LIMITED TO NEGLIGENCE), OR ANY OTHER GROUNDS.

**3.3.** The term of this User Agreement will begin on the date that You execute below and will expire on the second anniversary of such date, except that the confidentiality obligations set forth in Section 0.2 will survive such expiration. If You wish to continue to use the ICCB-L facility and have access to screening data generated at the facility by other users, You will need to execute a new User Agreement.

**3.4.** This User Agreement may not be assigned or transferred to anyone else. This User Agreement will be governed by and construed in accordance with the laws of the Commonwealth of Massachusetts, without regard to any choice of law principle that would dictate the application of the law of another jurisdiction. You consent to the sole jurisdiction of the state and federal courts sitting in the Commonwealth of Massachusetts, without restricting any right of appeal.

**3. The following conditions apply if You screen the ICCB-L Authenticated Traditional Chinese Herbal Extract Collection:**

**3.1.** The **Authenticated Traditional Chinese Herbal Extract Collection (ATCHEC)** is to be used only for (i) primary screening purposes and (ii) hit confirmation using the same assay procedures.

**3.2.** You will deposit your **ATCHEC** screening data into Screensaver the same as for other chemical libraries available to you at ICCB-L. However, unlike the other ICCB-L chemical libraries, results from your screen of the **ATCHEC** library will only be made available to You, ICCB-L staff, and authorized members of the Program that provided the extracts. They will not be shared with other ICCB-L screeners.

**3.3.** You will not analyze any of the Materials from the **ATCHEC** library to determine the chemical composition, formula, structure or properties of the Materials. Chemical or property analysis of active entities from the **ATCHEC** library will only be carried out in collaboration with authorized members of the Program, under a separate collaboration agreement. It is anticipated that the parties will discuss entering into such a collaboration agreement if the screening of the **ATCHEC** results in any meaningful discovery, relating to Materials, in order to further research such discovery.

**4. The following conditions apply if You screen any compounds provided by the NIH Molecular Libraries Program (MLP):**

**4.1.** You must sign a Material Transfer Agreement (MTA) governing Your use of compounds provided by the MLP (e.g., compounds from the ICCB-L MLP1 library). The Harvard Office of Technology Development has approved a MTA for use by Harvard and Harvard-affiliated investigators; this form is available from the ICCB-L. Investigators from other institutions should contact the ICCB-L for information on completing a MTA for access to these compounds.

**4.2.** The ICCB-L will work with You to establish a formal plan for screening MLP compounds. The plan will specify how many compounds will be screened and provide a timeline for completion of the primary screen. The plan will state all ICCB-L policies related to MLP compounds, including data deposition and cherry pick policies.

**4.3.** Data from the primary screen will be deposited in PubChem within 6 months of completion of the primary screen, with the option to place up to a one-year hold on public



display of the data via the PubChem interface. Cherry picks of MLP compounds may be requested. However, You will not receive cherry pick samples before Your primary screening data are deposited in PubChem. You may receive cherry picks immediately upon data deposition even if a one-year hold is implemented.

**4.4.** Confirmation data for the cherry picks will be deposited in PubChem within 6 months of receipt of cherry picks by You, again with the option to place up to a one-year hold on public display of the data via the PubChem interface. Confirmation data will consist minimally of a simple yes/no assessment of each cherry pick's activity in the original screening assay.

AGREED:

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Signature of Screening Facility User	Printed name	Date
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ACKNOWLEDGED AND AGREED:

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Signature of Screening Facility User's Principal Investigator (if applicable)	Printed name	Date
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Institution:

Address:

ACKNOWLEDGED AND AGREED: *[Applicable for users who are not employed by Harvard.]*

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Signature of Institutional Biosafety Official	Printed name	Date
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Institution:

Address:

Please e-mail signed (scanned) forms to: Jennifer Smith at [jennifer\\_smith@hms.harvard.edu](mailto:jennifer_smith@hms.harvard.edu). If necessary, forms may be faxed or sent by post to Dr. Jennifer Smith, Harvard Medical School, 250 Longwood Avenue, Seeley Mudd Building, Room 604, Boston, MA 02115; 617-432-5735 (tel), 617-432-6424 (fax).