Notes & Instructions for Recipient

Congratulations! You have been conditionally approved as a Recipient for the BU-CMD compound repository.

Final approval requires your Institution's execution of two types of non-negotiable Material Transfer Agreements governing the transfer of the materials: one to be executed between your institution and BU (called a BURTA), and an agreement between your institution and the external provider (s) (called an SPMTA) for each compound to be transferred to your institution.

Please read the following instructions and guidelines carefully. In order to complete this submission, we need a number of items from you:

Recipient checklist (3+ items):

- ✓ **Generic Assay Description**. Please provide us with a generic, non-confidential description of your assay that you are comfortable with us sharing openly with our depositors. They like to know where their compounds are going!

- ✓ A signed, fully executed **BU Recipient Transfer Agreement (BURTA)** between an authorized signatory at your institution and Boston University.

  The BURTA will be sent to your institution for e-signature upon receipt of your Generic Assay Description

- ✓ Signed, fully executed **Standard Provider Material Transfer Agreement Between Provider and Recipient (SPMTA)** with each provider.

  A set of SPMTAs will be sent to your institution for e-signature upon receipt of your Generic Assay Description

What to expect from us:

- We will prepare and ship screening quantities of compounds according to the format you specified in your Questionnaire submission. We will contact you for any further information needed.

- Please bear in mind that collection plating is a labor-intensive process that can take several weeks.
- When plating is completed, we will notify you *via* email and ship the plates to the address specified in your BURTA agreement. We will notify you via email with tracking information and digital platemap(s).
- **Safety precautions:** The shipment you receive will also contain a Material Safety Data Sheet (MSDS) that contains details on safe handling, storage, and disposal of the screening collection compounds. Please also note the following:
    - The compounds that you receive are of an experimental nature, and may have hazardous properties.
    - Potential exposures should be controlled through the implementation of prudent laboratory practices for handling, storage, and disposing of chemical substances of unknown toxicity.
    - All personnel handling the screening collection should be properly trained in Chemical Safety by your institution's Health & Safety Office, and should be familiar with your institution's Chemical Hygiene Plan.
    - All personnel handling the screening collection should wear the appropriate personal protective equipment for handling chemicals of unknown toxicity.
    - The screening collection should be stored in a refrigerator or freezer in your laboratory that is designated for chemical storage purposes.
    - Please consult with your institution's Health and Safety office and Chemical Hygiene plan for additional state-specific regulations and guidelines for chemical handling and disposal.

What we expect from you:

First, read the BURTA and SPMTA carefully! These documents outline your legal responsibilities as a recipient of our collection.

- Our most important expectation is that you screen our compounds, and let us know what you find!

- When you report screening results to us, lists of hits are good, but lists of hits plus raw data is better. Please aim to send along raw data files (as Excel or CSV) alongside your list of the most promising hits. This enables us to archive activity data for all compounds in our repository, and let our depositors know what kinds of activities have been seen (or not seen) with their compounds.
    - Our activity database is secure, password-protected, and accessible only to BU-CMD leadership.
    - We will not redistribute your raw data without your consent.
    - We will not inform Depositors of compound activity without simultaneously notifying you.
    - We may inform Depositors of lack of activities (negative results) without notifying you. These disclosures will only be performed in broad terms, using your provided Assay Generic Description.
    - **Note on cytotoxicity control data:** If you are running cellular assays with a control readout for cytotoxicity, we may use solely the control results to conduct broad cytotoxicity assessments for collection molecules. This will be performed in a completely anonymous manner, and we will not incorporate any screening results or assay descriptions in this analysis. If you object to this, please notify the Assistant Director Lauren Brown (brownle@bu.edu) in writing prior to signing the BURTA.

- Once hits have been identified, the next step is validation. At the BU-CMD, a hit is considered "validated" when its activity has been replicated with a freshly-QCed, resupplied aliquot of the sample. Your list of hits will be used to generate a validation cherrypick, which may be supplemented with "near neighbors" of interest, dependent on availability.

- After validation, we will collaboratively determine next steps forward for the hit compound(s). Please be prepared to outline for us your secondary assay plan for hits, and the quantity of compound that you will require for these assays.

- Please note that for validated hits that were submitted by external Depositors, upon validation we will promptly put you in contact with the Depositors and disclose the hit status to them. It is our hope that this will seed a future collaboration between you and the Depositors, with or without BU-CMD involvement.

Best practices in dealing with compound structures – an important note about disclosure

Please, **do not publicly disclose "hit" structures with their associated activity** without first consulting with both the BU-CMD and the chemist who deposited the compound.

What constitutes public disclosure?

"Public disclosure" can include posters, papers, abstracts, theses, lectures, websites, etc. Even grant proposals, which can be subject to FOIA inquiry when funded, require special precautions for protecting IP-sensitive information.

Why is this important?

Premature public disclosure of the structures and activity of biologically active compounds can compromise our collective ability to patent promising drug leads, their derivatives and analogs.

We as academics are often motivated more by the potential impact of our scientific results than their potential for profit. However, the unfortunate reality of drug discovery is that if a molecule is not IP-protected, it is not going to be developable as a drug. In order to maximize potential for your research to meaningfully impact those who suffer from disease, we are obligated to take adequate precautions around possible IP.

How should we move forward when a hit is identified?

The BU-CMD will work collectively and transparently with Depositors and Recipients to determine a responsible and appropriate path forward that adequately balances our dual (and sometimes dueling) obligations to promptly publish our results while protecting the IP of promising drug leads.

In keeping with this, we strongly request that no public disclosure of small molecule bioactivities that have been identified through our CLC network screens be made without clear, unambiguous consent of all parties (Depositor, Recipient, and BU-CMD).