Title: **Compound Registration for CSAR project – Standard Operation Procedures**

Rev. # : **Version 1**

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Author: **James B. Dunbar Jr. and Scott Larsen**

1. General

1.1. Information is to be stored on the CSAR research computer, designated as ale.phar.umich.edu, in the account provided to each member. The login is via your UM uniqueid and your Kerberos password.

1.2. Information is backed up daily (keep 7), weekly (keep 4), monthly (keep 12) and yearly (keep 1) via rsnapshot (rsync) to another server located on north campus designated as stout.phar.umich.edu. This is a disk to disk backup. Data recovery is via a sysadmin request (direct requests to Jim Dunbar).

1.3. The information associated with compound registration will be that of minimal publication quality level.

2. Information in master Excel Spreadsheet

2.1. The master excel spreadsheet is currently maintained by Jeanne Stuckey and updated by her upon registration. Jeanne is currently providing the barcode. This will change and the change will be reflected in a new revision of the document. The location of the master spreadsheet will be on the server ale.phar.umich.edu in the directory: /data/people/master_chemical_inventory and readable by all.

2.2. Information stored in the master registration spreadsheet is: CS<barcode number>, notebook number, name of chemist, principal investigator, organization, and physical location of the compound specific files on the disk. Column headers are as follows: Barcode Number, Notebook Number, Chemist, Principal Investigator, Organization, File Location, and Date of Entry.

2.2.1. The physical location is as described in the following example: /data/people/uniqueid/series_name/CS<barcode number>. The series name is to be mutually agreed up by the chemists and submitting entities, but specifically to include Hollis Showalter, Scott Larsen and James Dunbar. The series name to be of a form <protein target>_<defining chemical fragment>.

2.2.2. The designation of an *alpha numeric* entry for the registration number, as an example CS000001, maintains the designation upon moving between Excel and other software. The compound designator is always to be treated as a character string.

2.2.3. Organization is defined as the institution or company name, such as University of Michigan or Glaxo Smith Kline.

3. Detailed information needed for compound registration

3.1. Submitter name

3.2. Principal Investigator name (lab head)

3.3. Barcode (issued at time of registration)

3.4. Notebook reference

3.5. Experimental procedure for preparation (three options)

3.5.1. Literature reference may be cited if exact procedure is described

3.5.2. A general procedure (JOC style) may be described for compounds prepared as part of a library synthesis. For novel procedures, the general method should be further exemplified with one specific example including scale of reaction and yield. For other members of the library, only yields should be listed. Physical (e.g., mp) and spectroscopic (nmr, ms) data should be listed for any new compounds and prior citations to known compounds provided. If a library is made by a known general procedure, it may be cited. In this case, yields and physical data should be reported out according to the above criteria. ,

3.5.3. For singleton synthesis, a detailed procedure (JOC style) is required if the procedure is unique and not described in the literature. Otherwise, citations to known procedures and/or compounds should be made.

3.5.4. For 3.5.2 and 3.5.3 above, *the procedures must include either refs to required synthetic intermediates that are in the literature, or detailed experimental procedures (and data) for intermediates that are novel.*

3.6. Analytical data

3.6.1. Purity (%) and method of determination (NMR, HPLC or combustion analysis) are required for all compounds

3.6.2. Spectral (NMR, MS) and any other data (HPLC, TLC, combustion analyses) must be written up in publication-ready format (JOC style) and be included in the experimental procedure. *If these data are available in the literature for a compound, it is sufficient to cite that the NMR and MS data agree with what is reported*.

3.6.3. Regardless of whether a compound is reported in the literature or not, the NMR and MS spectra for every compound must be scanned to create .pdf files, which will be linked into the CSAR database. HPLC traces should also be scanned if available.

3.7. Experimental procedures and analytical data for any series should be checked by the appropriate PI prior to compound registration.

3.8. Chemical structure file (2D) for each compound in the form of a Chemdraw .cdx file. The drawing will include stereochemistry assignments where appropriate.