Tutorial 13: Simple Tox Format
SimpleTox for Toxicogenomics Study

• Used directly for uploading data from toxicogenomics experiments (non-clinical data and clinical data)
  http://www.cdisc.org/models/send/v1.4/index.html

• Rationale behind SimpleTox
  – To capture essential information from microarray and toxicity studies to enable cross-study analysis
  – To mimic the way biologists manage & organize data
  – To be compliant with MIAME and SEND

• Format
  – Excel spreadsheet format
  – Contains required and optional fields
  – Customization: users are able to add new fields
  – Searchable
SimpleTox Overview

How to access SimpleTox in ArrayTrack:
Click “Studies…” button to bring out the window below.

Select one study, the experiments that reference the selected Study will be shown below.

Search data by study and individual.

These two tabs show that there is one experiment associated with the study above, and there are 59 hybridizations for this experiment.
SimpleTox Overview

(Continued.)
Click the “Hybs” tab to display information about the 59 hybridizations in this experiment.
SimpleTox Overview

Highlight the exp and click “Select Exp Dataset” button will select all the data (or just raw/normalized data) in the data panel for data analysis (see the screen shot on the next slide).

You can select the study named “Simple ToxFormat Demo”, then click “View Observations” to view the detail of the study including sample info and toxicological info. (See the observation viewer on the next slide).
SimpleTox Observation Viewer

Switch to study summary domain

User can also change the display of column names
Access SimpleTox information from microarray database

Data analysis

Group data according to sample info and toxicological info.
Batch Import – Simple Tox Format

Right-click the experiment, choose “Batch Import Data – Simple Tox Format”

Click Browse button to locate the Simple Tox file and data files directory. The next slide shows an example of a Simple Tox table file.
Batch Import – Simple Tox Format

This is an example of a Simple Tox file (this file can be downloaded from the ArrayTrack help pull-down menu.). Users can base their own Simple Tox files on this example. Just make sure that your column titles are exactly same as this template. You are allowed to add new columns, however using the existing columns will make future analysis across studies simpler.

The next slide shows a table that explains the meaning of the column names. The order in which a column appears doesn’t matter.
## SimpleTox Format Explanation

<table>
<thead>
<tr>
<th>SimpleTox Column Head</th>
<th>Description</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Institution</td>
<td>Laboratory or institution name</td>
<td>NCTR/FDA, EPA</td>
</tr>
<tr>
<td>DataFile</td>
<td>Microarray data file</td>
<td>GSM142129.CEL</td>
</tr>
<tr>
<td>HybName</td>
<td>User specified identifier for a hybridization name</td>
<td>APAP_D100_T6_Jun04; APAP_D0_T6_Jun04</td>
</tr>
<tr>
<td>SampleName</td>
<td>Sample name</td>
<td>APAP_Dose100_Time6; APAP_Dose0_Time6</td>
</tr>
<tr>
<td>Array_ID</td>
<td>User-specified identifier for a hybridization</td>
<td>1,2,3 … or p1002356</td>
</tr>
<tr>
<td>Label</td>
<td>RNA label reagent</td>
<td>Biotin; Cy3</td>
</tr>
<tr>
<td>ArrayType</td>
<td>Array type</td>
<td>Affymetrix Mouse 430_2</td>
</tr>
<tr>
<td>Subject_ID</td>
<td>Subject identifier</td>
<td></td>
</tr>
<tr>
<td>StudyTitle</td>
<td>Study title</td>
<td>6 days repeating toxicity study</td>
</tr>
<tr>
<td>Tech_Rep</td>
<td>Technical replicates; microarray specific</td>
<td>A, B or C; 1,2, or 3</td>
</tr>
<tr>
<td>Bio_Rep</td>
<td>Biological replicates</td>
<td>A, B or C; 1,2, or 3</td>
</tr>
<tr>
<td>HybDate</td>
<td>Hybridization date</td>
<td>2/25/2007</td>
</tr>
<tr>
<td>StudyType</td>
<td>Study type</td>
<td>Single Dose Toxicity or Repeat Dose Toxicity</td>
</tr>
<tr>
<td>Compound</td>
<td>Compound name</td>
<td>Carbon Tetrachloride; Acetaminophen</td>
</tr>
</tbody>
</table>

**Red-colored** fields are required, while **black-colored** fields are optional. If you don’t have an Array_ID, subject_ID can be repeated and used as the Array_ID.
Batch Import – Simple Tox Format

If the array type specified in the Simple Tox file does not exactly match an array type in ArrayTrack’s Chip library, choose the correct array type from the drop-down menu.
Batch Import – Simple Tox Format

Importing hybridization
RT_0_13_22_Lung_CornOil_Mouse430_2_IMFIN0023_8 792...
Inserting intensity data...

Processing hybridization RT_0_13_22_Lung_CornOil_Mouse430_2_IMFIN0023
Inserting sample "RT_0_13_22_Lung_CornOil" for hybridization RT_0_13_22_L...
OK Inserted sample "RT_0_13_22_Lung_CornOil"
No sample # 2 specified
Looking for existing hybridization record for "RT_0_13_22_Lung_CornOil_Mouse..."
Inserting hybridization record for "RT_0_13_22_Lung_CornOil_Mouse430_2_IMF..."
OK Inserted new hybridization "RT_0_13_22_Lung_CornOil_Mouse430_2_IMFIN002..."
Converting cell "GSM142128.CEL" to probe-set file...
Batch Import – Simple Tox Format

Import Summary
Import of 10 hybridizations and 10 toxicological observations completed without error.

Detailed Import Log

Processing hybridization
RT_0_13_22_Lung_CornOil_Mouse430_2
RT_0_13_24_Lung_CornOil_Mouse430_2
RT_0_13_25_Lung_CornOil_Mouse430_2
RT_0_13_27_Lung_RodentChow_Mouse43
RT_0_13_28_Lung_RodentChow_Mouse43
RT_0_13_29_Lung_RodentChow_Mouse43
RT_2000_13_12_Lung_ethylene_diamine
RT_2000_13_14_Lung_ethylene_diamine
RT_2000_13_15_Lung_ethylene_diamine
RT_2000_13_2_Lung_Naphthalenediamine

Batch import is successfully finished.
Delete Data

To delete SimpleTox data you have imported, you need to delete the experiment first and then delete the study. Double-click the experiment name in the data panel to bring out the Input Form, then click “Delete Exp” button.

You will be asked the following question, click “Yes” button to permanently delete the experiment.
Delete Data

After the experiment is deleted, you need to delete the study. Select the study, right-click, Choose “Delete Studies”.

Click the “OK” button.