

# **User Manual**

## **Integration of LEAP Shell DART Control and MSRedux-XI in the Analyst Context**

**Version 1.0**



**IonSense, Inc.  
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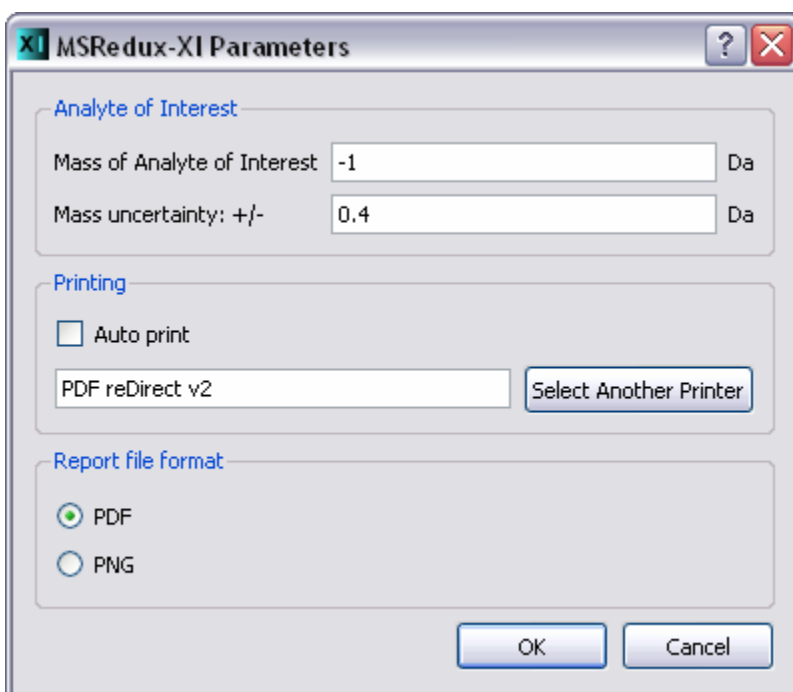
# Quick Start Guide for Using Automated, Real-time MSRedux-XI in the LEAP Shell Context

## *Install MSRedux-XI*

Follow the *Quick Start Guide for MSRedux-XI* for downloading, installing, licensing and running MSRedux-XI.

## *Setting the Default MSRedux-XI Parameters for the Automated Mode of MSRedux-XI*

Be sure to manually set in “MSRedux-XI Parameters” the settings that you wish to execute in the automation/non-interactive mode of MSRedux-XI.



Exit the MSRedux-XI user interface by selecting:  
**File->Exit**



When you see the screen shown above upon exiting MSRedux-XI, the MSRedux-XI Parameters set manually will be saved as the defaults for the automation/non-interactive mode of MSRedux-XI. Click “Yes” to exit.

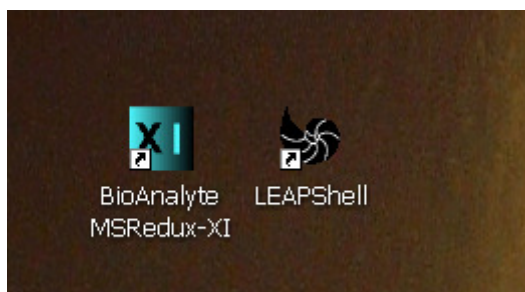
## ***Install LEAP Shell for AutoDART***

Follow the *LEAP Shell 3 for AutoDART Manual* for downloading, installing and licensing instructions and for general LEAP Shell settings.

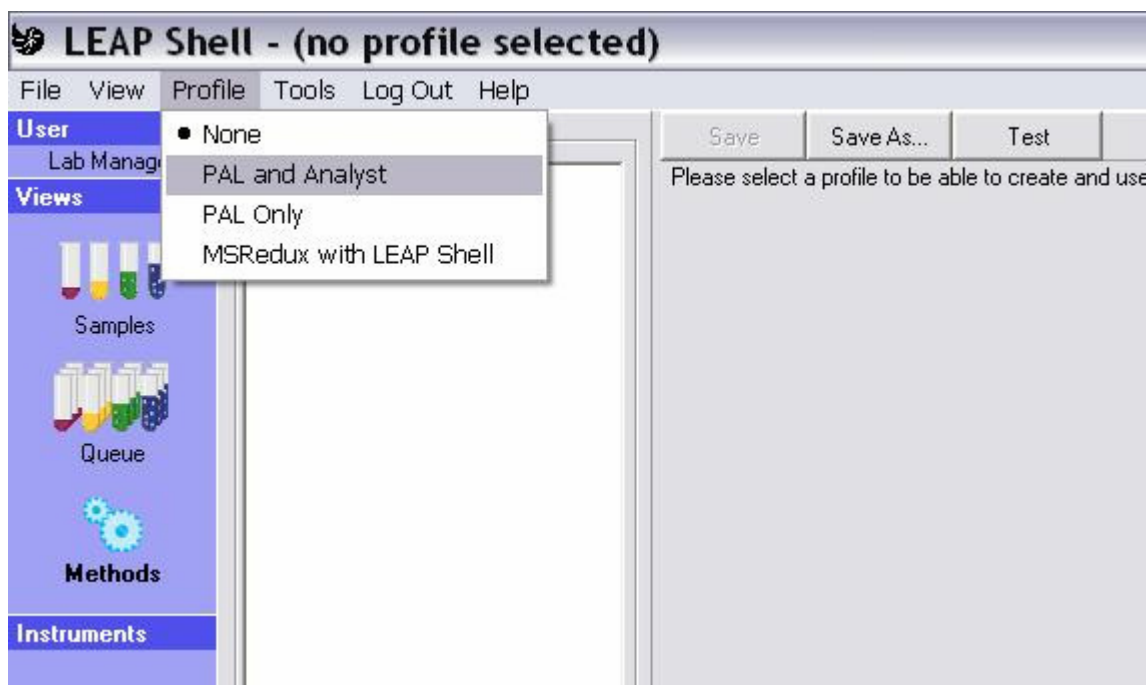
**Note:** A PDF copy of the *LEAP Shell 3 for AutoDART Manual* can also be found in the contents of the LEAP Shell installation CD.

## ***Setting LEAP Shell up for the Analyst Context***

Start LEAP Shell by double clicking the “LEAPShell” icon located on the Desktop.



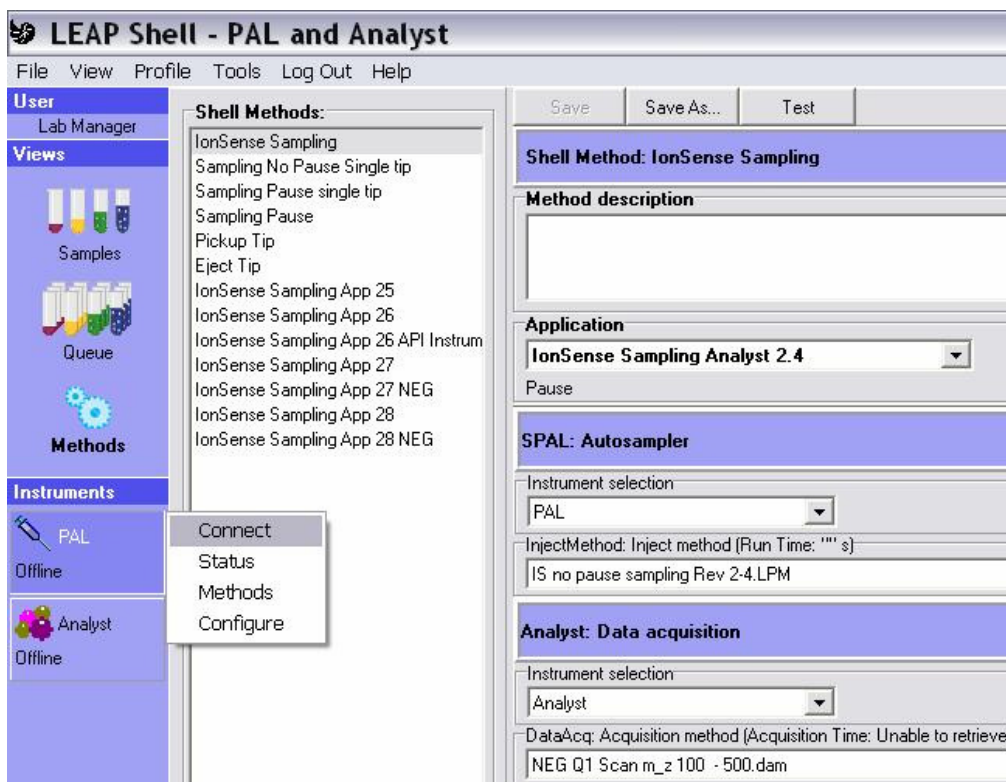
Once LEAP Shell opens, choose under “**Profile**” the “**PAL and Analyst**” profile.



## Connecting to the PAL

In the header next to “LEAP Shell” it should now read “**PAL and Analyst**” for the “**PAL and Analyst**” profile that was just selected.

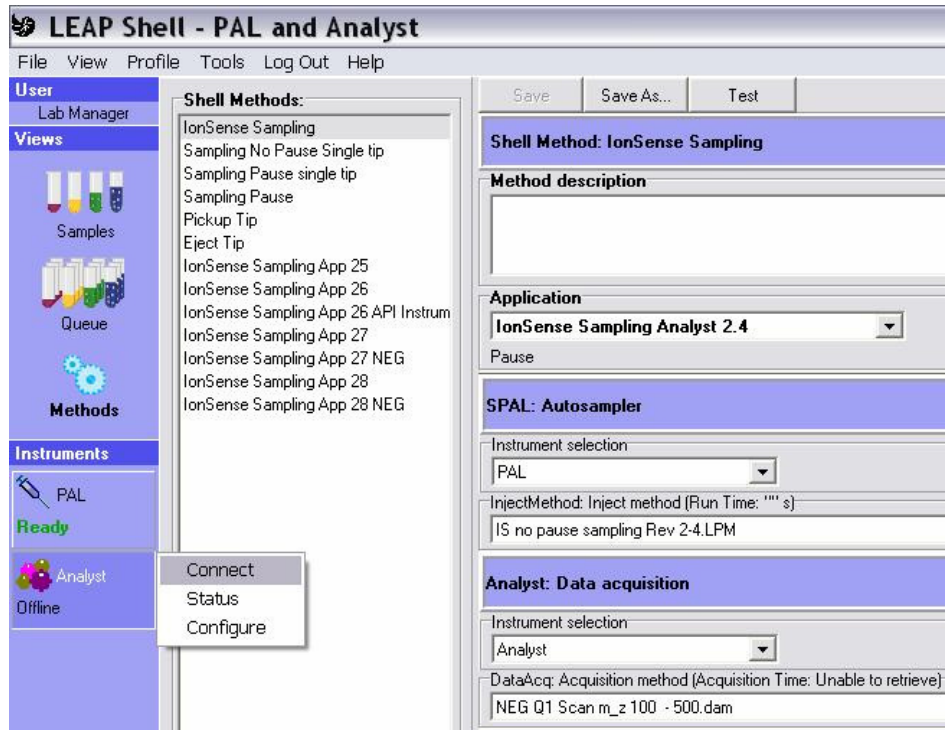
Now connect to the **PAL** by left clicking on the **PAL** icon in the “**Instruments**” bar and then clicking on “**Connect**”. Within a few seconds the word “**Ready**” in green text should appear.



**Troubleshooting:** If you are having difficulties connecting to the PAL, first make sure that the PAL power supply has been switched on and that the PAL serial cable is connected to the PC that will be controlling the PAL. If you still cannot connect to the PAL restart the LEAP Shell software and then try again to connect to the PAL.

## Connecting to Analyst through LEAP Shell

Connect to Analyst by left clicking on the “Analyst” icon found under “Instruments” in LEAP Shell and then click on “Connect”. In a few seconds the Analyst status will change from “Offline” to “Standby”.

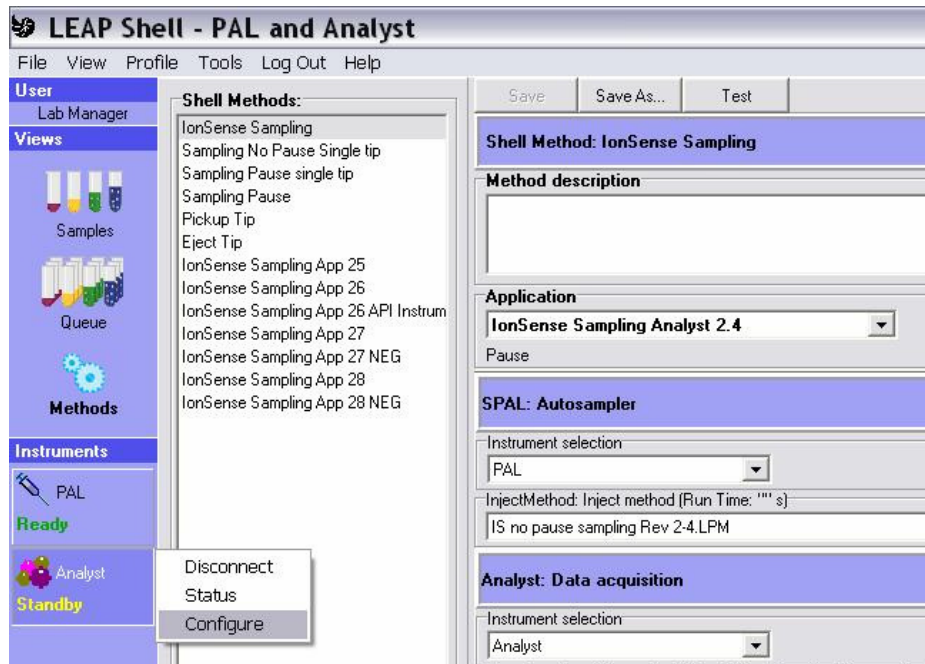


PAL in “Ready” state and Analyst in “Standby”.

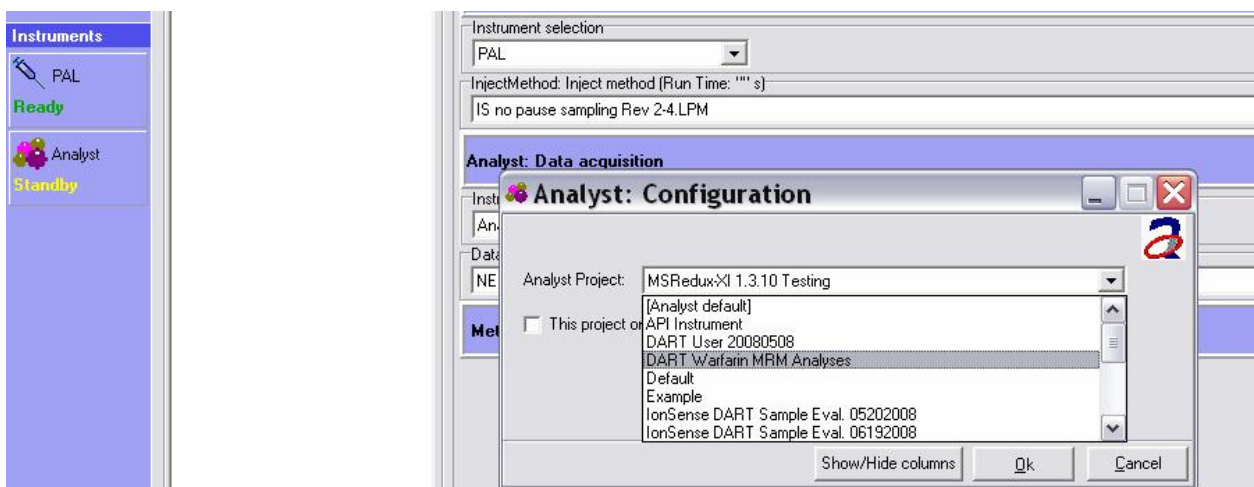


## Configuring to an Analyst Project through LEAP Shell

Left click again on the “Analyst” icon and select “Configure”.



In the “Analyst: Configuration” dialog box that appears, configure to the “Analyst Project” that will contain the “Analyst Acquisition Method” you wish to use to collect the data. Select the desired “Analyst Project” from the drop down menu and click “Ok” to save the changes and exit from the configuration.



## Creating a LEAP Shell Method to Include an Analyst Acquisition Method

For general questions about creating a Shell Method refer to the *LEAP Shell 3 for AutoDART Manual*.

The Analyst specific sections in the LEAP Shell Method are the “**Analyst: Data acquisition**” section and the “**DART Warm-up Time (min)**” that appear at the bottom of the page.

In “**Analyst: Data acquisition**” section the “**Instrument selection**” will be “**Analyst**” and the Analyst Acquisition Method will be chosen from the drop down box labeled “**DataAcq: Acquisition method**”.

The screenshot shows the configuration window for the SPAL: Autosampler. It is divided into two main sections. The top section, titled "SPAL: Autosampler", has a blue header and contains an "Instrument selection" dropdown menu set to "PAL". Below it is a text field for "InjectMethod: Inject method (Run Time: "" s)" with the value "IS no pause sampling Rev 2.4.LPM". To the right of this field are "Default" and "Show Params" buttons. The bottom section, titled "Analyst: Data acquisition", also has a blue header and contains an "Instrument selection" dropdown menu set to "Analyst". Below it is a text field for "DataAcq: Acquisition method (Acquisition Time: 20.10 s)" with the value "Sciex Test Meth.dam". A dropdown menu is open below this field, showing "NEG Q1 Scan m\_z 100 - 500.dam" and "Sciex Test Meth.dam". To the right of this field are "Default" and "Show Params" buttons.

The “**DART Warm-up Time (min)**” feature allows the user to set a fixed time interval for the DART to heat at the beginning of EVERY sample batch submitted to the LEAP Shell Sample Queue. The default time is set to 0 minutes.

The screenshot shows the configuration window for the Analyst: Data acquisition. It has a blue header and contains an "Instrument selection" dropdown menu set to "Analyst". Below it is a text field for "DataAcq: Acquisition method (Acquisition Time: 20.10 s)" with the value "Sciex Test Meth.dam". To the right of this field are "Default" and "Show Params" buttons. The bottom section, titled "Method Parameters", has a blue header and contains a text field for "DART Warm-up Time (min)" with the value "3.00" and a spinner control.

When a “**DART Warm-up Time**” is set the following will take place:

- **DART Control** will automatically be turned “**ON**” by LEAP Shell at the beginning of EVERY sample batch in the LEAP Shell Queue and LEAP Shell will wait for the set warm-up time.
- The **DART status** automatically changes to “**RUN**”.
- The **DART heater** is automatically turned “**ON**” and set to the “**Run Time**” heater temperature set through the DART Method.
- The **DART “Run Time” gas** is automatically selected.

**Note:** These events also occur even if no DART Warm-up Time is set, e.g. set to 0 min.



## Setting up the LEAP Shell Sample List to Acquire Analyst Data

The user has two options to create a sample list to run in LEAP Shell:

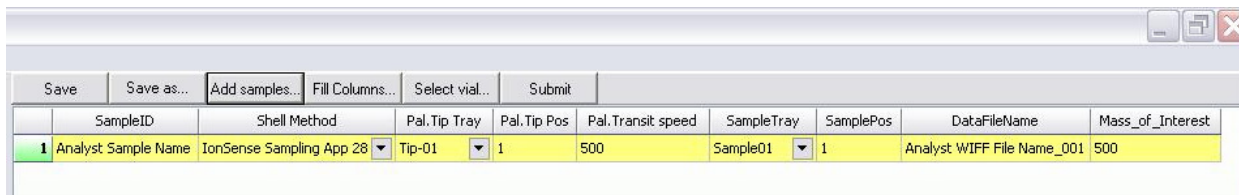
1. Directly within LEAP Shell by filling in the required fields
2. By importing a file into LEAP Shell

***This sample list set-up assumes 1 sample analysis (1 data acquisition) per Analyst .wiff file.***

### Creating a Sample List Directly in LEAP Shell for Analyst Data

The first option is straight forward. Shown in the image below are the generic fields the user will need to fill in when creating a sample list directly in LEAP Shell for Analyst data acquisition.

- The LEAP Shell “SampleID” will be the “Analyst Sample Name”
- The “DataFileName” will become the Analyst .wiff file name
- The “Mass\_of\_Interest” column is reported to MSRedux-XI for the data processing. The mass of the analyte in Daltons (not the m/z value) should be entered here.
  - **Note:** A value of “-1” may also be entered in this “Mass\_of\_Interest” field provided that a molecular formula for the analyte of interest is contained within the sample information. The only way that the user may create a custom column labeled “Formula” is to import a sample list into LEAP Shell. This feature is explained in greater detail in the *Importing a Sample List into LEAP Shell from a File* section of this manual.



SampleID	Shell Method	Pal.Tip Tray	Pal.Tip Pos	Pal.Transit speed	SampleTray	SamplePos	DataFileName	Mass_of_Interest	
1	Analyst Sample Name	IonSense Sampling App 28	Tip-01	1	500	Sample01	1	Analyst WIFF File Name_001	500

**Note:** There is a **limit of 80 characters total** for the length of the “DataFileName” entered in the LEAP Shell sample list plus the name of the **Analyst Project** that LEAP Shell is configured to. If the combination of these two names exceeds 80 characters in length the quality of the MSRedux-XI printout will be reduced.

## Importing a Sample List into LEAP Shell from a File

The sample list file to be imported into LEAP Shell may be saved in any of the following formats:

- Tab delimited (text) file
- CSV file
- Microsoft Excel file
- XML file

Pictured below is an example of a CSV file opened in OpenOffice.org's Calc program. The general components found in the LEAP Shell sample list are contained in the CSV file, with the addition of the "Formula" custom column that has been added by the user.

	A	B	C	D	E	F	G	H
1	SampleID	Pal.Tip Pos	Pal.Tip Tray	Analyst.DataFileName	SampleTray	SamplePos	Formula	Mass of Interest
2	Analyst Sample Name 1	1	Tip-01	Analyst WIFF File Name_001	Sample01	1	C7H6BF303	206.04
3	Analyst Sample Name 2	2	Tip-01	Analyst WIFF File Name_002	Sample01	2	C7H6BF303	206.04
4	Analyst Sample Name 3	3	Tip-01	Analyst WIFF File Name_003	Sample01	3	C7H6BF303	206.04
5	Analyst Sample Name 4	4	Tip-01	Analyst WIFF File Name_004	Sample01	4	C7H6BF303	206.04
6	Analyst Sample Name 5	5	Tip-01	Analyst WIFF File Name_005	Sample01	5	C7H6BF303	206.04
7	Analyst Sample Name 6	6	Tip-01	Analyst WIFF File Name_006	Sample01	6	C7H6BF303	206.04
8	Analyst Sample Name 7	7	Tip-01	Analyst WIFF File Name_007	Sample01	7	C7H6BF303	206.04
9	Analyst Sample Name 8	8	Tip-01	Analyst WIFF File Name_008	Sample01	8	C7H6BF303	206.04
10	Analyst Sample Name 9	9	Tip-01	Analyst WIFF File Name_009	Sample01	9	C7H6BF303	206.04
11	Analyst Sample Name 10	10	Tip-01	Analyst WIFF File Name_010	Sample01	10	C7H6BF303	206.04
12	Analyst Sample Name 11	11	Tip-01	Analyst WIFF File Name_011	Sample01	11	C7H6BF303	206.04
13	Analyst Sample Name 12	12	Tip-01	Analyst WIFF File Name_012	Sample01	12	C7H6BF303	206.04
14	Analyst Sample Name 13	13	Tip-01	Analyst WIFF File Name_013	Sample01	13	C7H6BF303	206.04
15	Analyst Sample Name 14	14	Tip-01	Analyst WIFF File Name_014	Sample01	14	C7H6BF303	206.04

**Note:** The header for the "Formula" column can only contain the word formula as MSRedux-XI will only recognize entries in a column labeled with the word formula. Formula may be entered in the following formats: "Formula", "FORMULA", or "formula". For example, if the user labels the custom column "Chemical Formula" MSRedux-XI will not process any of the formulas in that sample list.

## ***The Chemical “Formula” Feature of MSRedux-XI***

In order for MSRedux-XI to process a chemical formula entered into the LEAP Shell sample list, the value “-1” must be entered into the “Mass\_of\_Interest” column for the each sample that contains chemical formula information. The “-1” tells MSRedux-XI to look for a chemical formula and use it to calculate a mass.

In the case that both a chemical formula and a theoretical mass of interest are entered into the LEAP Shell sample list, MSRedux-XI will use the mass of interest to determine the presence of the analyte of interest and the chemical formula is extra information.

If you select “-1” for a mass of interest, MSRedux-XI will look for a chemical formula in the wiff file and will calculate the mass of interest based on the formula. The formula should be written in with element names starting with capital letters. Two-letter elements should have lower case second letters. Number characters representing stoichiometry should follow the element. Omit all non alpha-numeric characters, viz., omit spaces, underscores, dashes, etc. Order of elements is not important. For instance, ethanol could be represented as

C2H6O

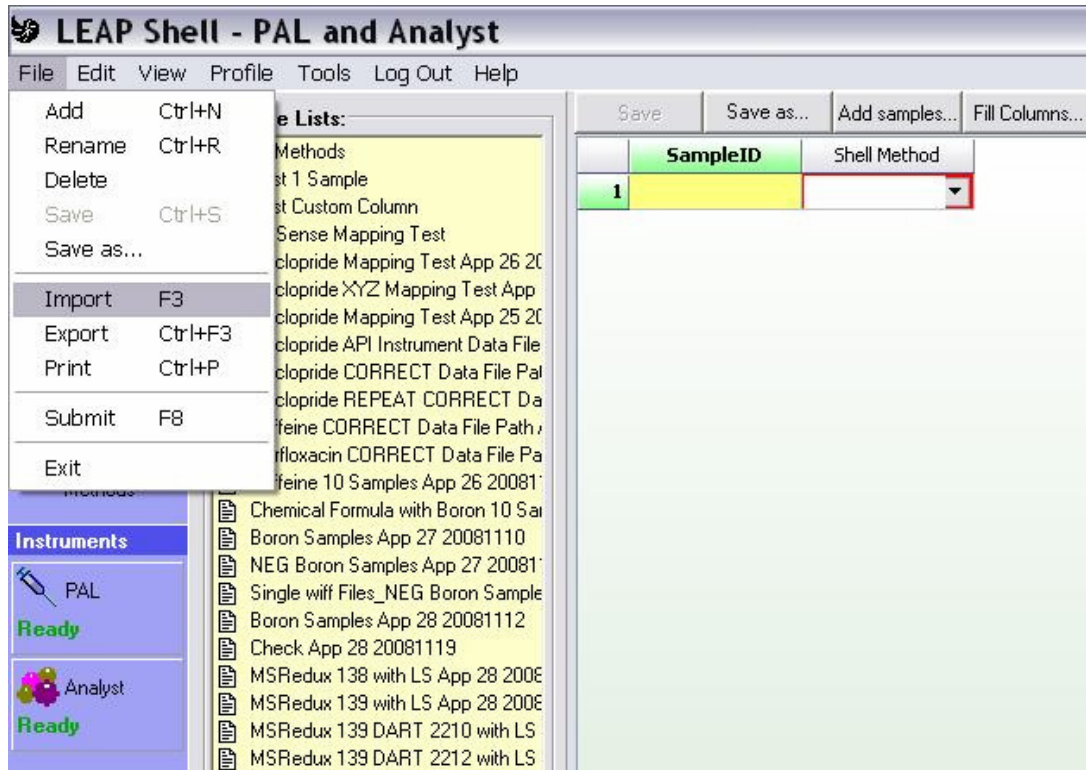
or

CH3CH2OH

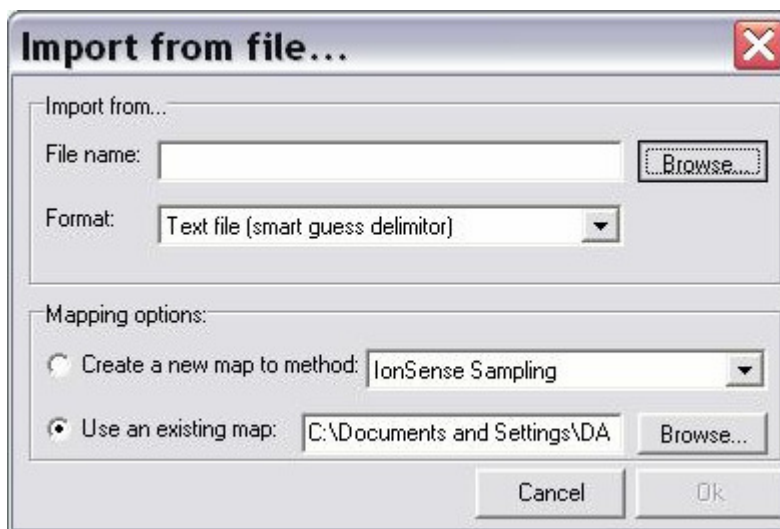
Sodium must be “Na” and never “NA”.

## Steps to Importing a Sample List into LEAP Shell from a File

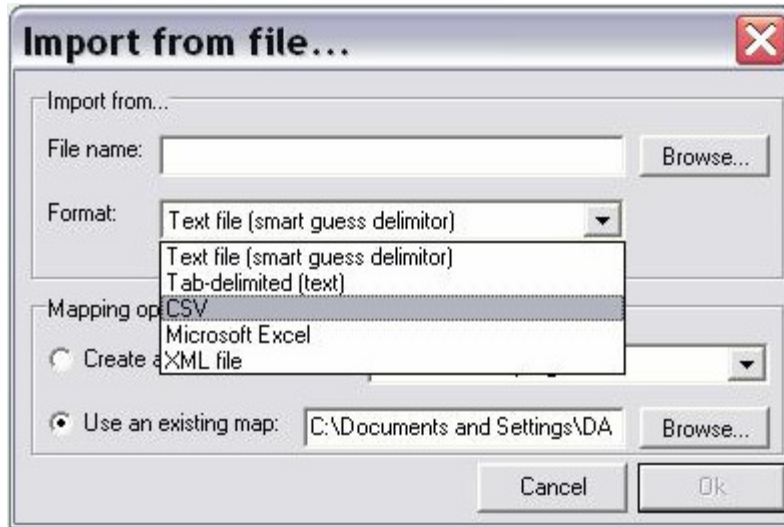
From the “**Samples**” Sample List view in LEAP Shell, the “**Import**” feature is found under “**File -> Import**” or can be accessed directly by hitting “**F3**” on the keyboard.



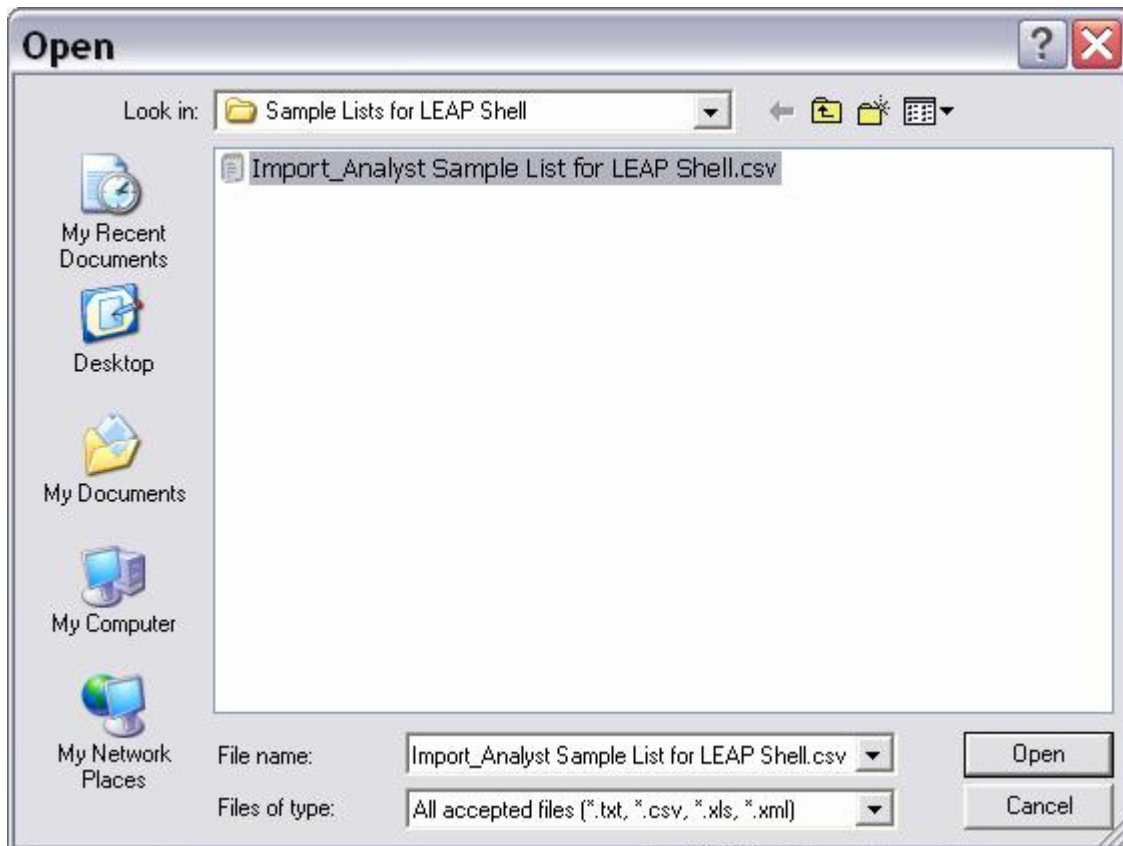
When the user engages the “Import” feature of LEAP Shell the “Import from file...” dialog box will appear on screen.



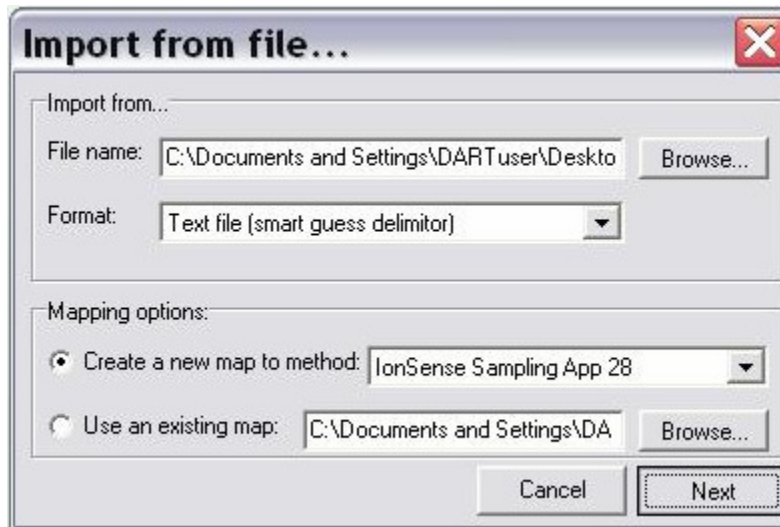
In this dialog box, the user can immediately select the “**Browse**” button leaving the default setting for the file format as “Text file (smart guess delimiter)” and lookup the desired file. The user may want to select the desired file’s format before browsing for the file to narrow down the number of possible files to choose from.



The image below shows the case where the user has left the default setting for the file format as “Text file (smart guess delimiter)” and began searching for the CSV file.



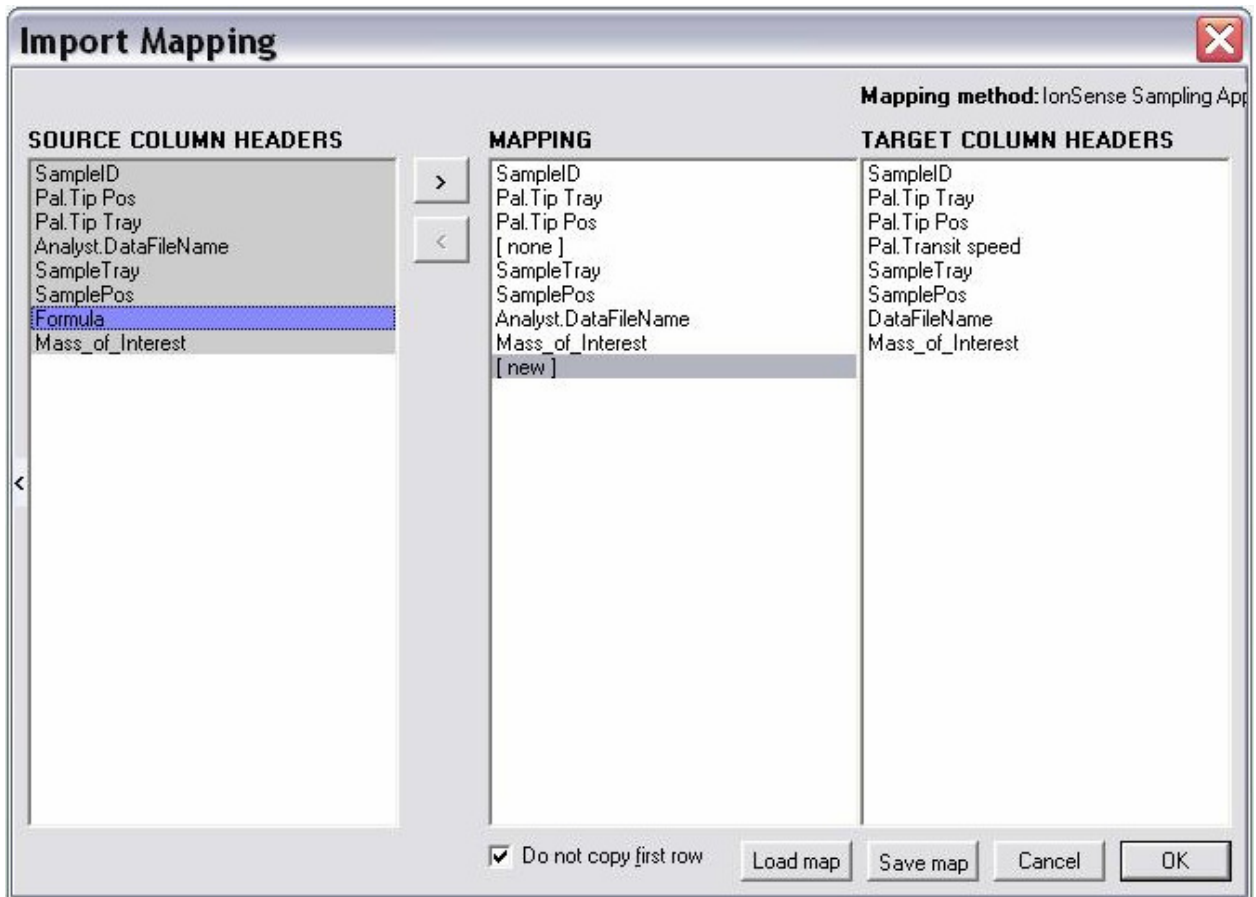
Once the desired file has been selected through the file browser, the user must select a mapping option to link the external sample list file to the LEAP Shell sample list layout.



To begin the mapping, select the **“Create a new map to method”** option, which will create a mapping that is specific to a LEAP Shell Method for the desired import file. Select a LEAP Shell Method and click **“Next”** to continue.

If a mapping file has previously been created and saved for the type of sample list that will be imported into LEAP Shell then the **“Use an existing map”** mapping option may be selected. Click **“Next”** to continue.

An “Import Mapping” window will appear after clicking on “Next” in the “Import from file...” dialog box. First begin mapping the non-custom “Source Column Headers” with their LEAP Shell “Target Column Headers” counterparts.

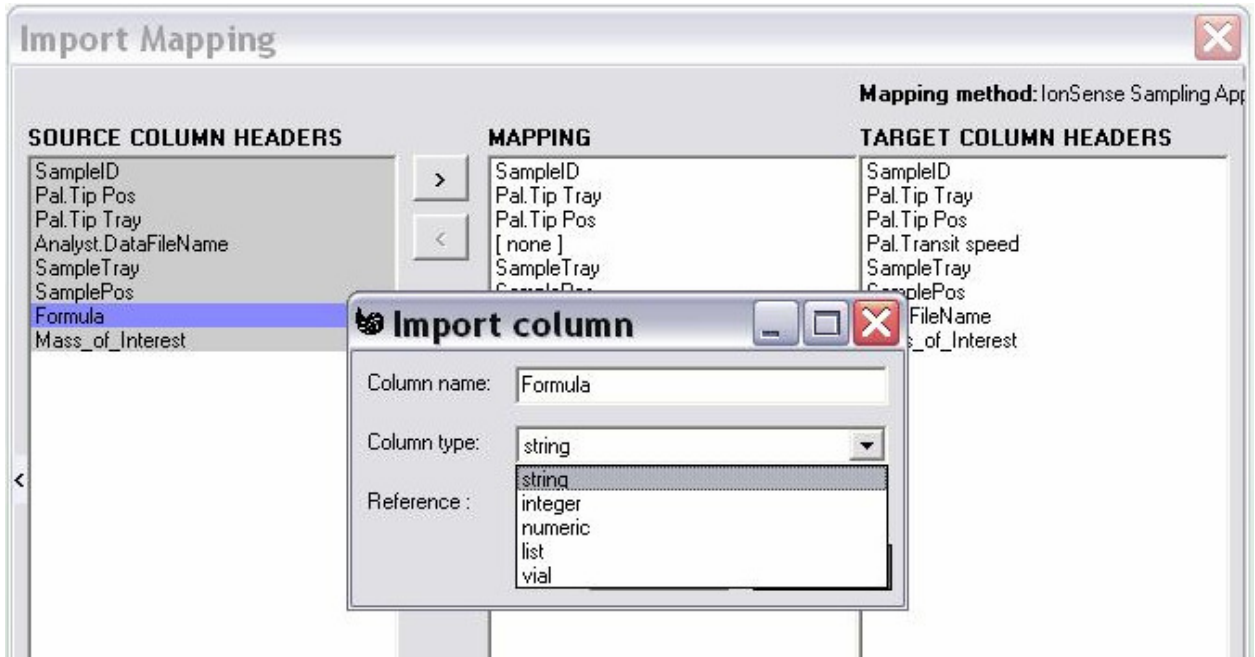


**Note:** When creating a sample list to import into LEAP Shell the mapping process can be simplified if the user keeps the same column naming in their document as there is in the LEAP Shell sample list for the generic columns, such as “SampleID” and “Pal.Tip Tray”.

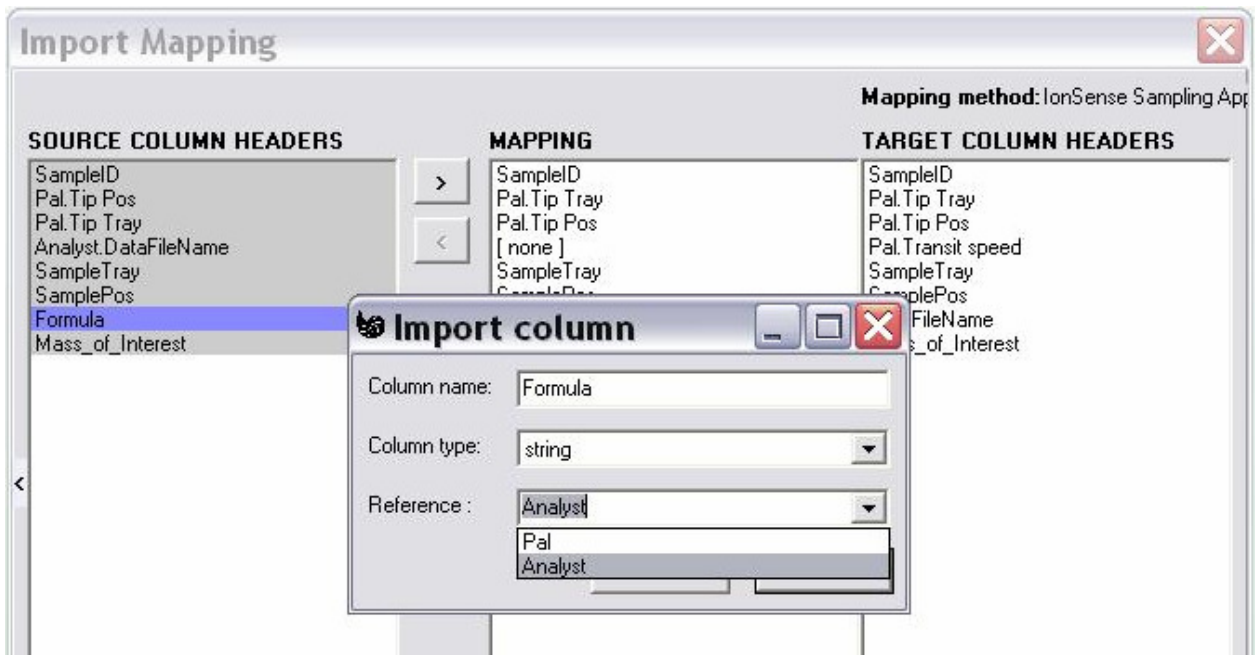
By keeping this continuity you can simply double click on each of the column names under “Source Column Headers” that directly match one of the LEAP Shell “Target Column Headers” to add them into the center “Mapping” column.



To map a custom column into a LEAP Shell sample list map it to the “new” option in the “Mapping” column. This will trigger the “Import column” dialog box to appear. The name of the custom column will appear in the text field for “Column name” as it was entered into the file that is being imported. For the column type select “string”.

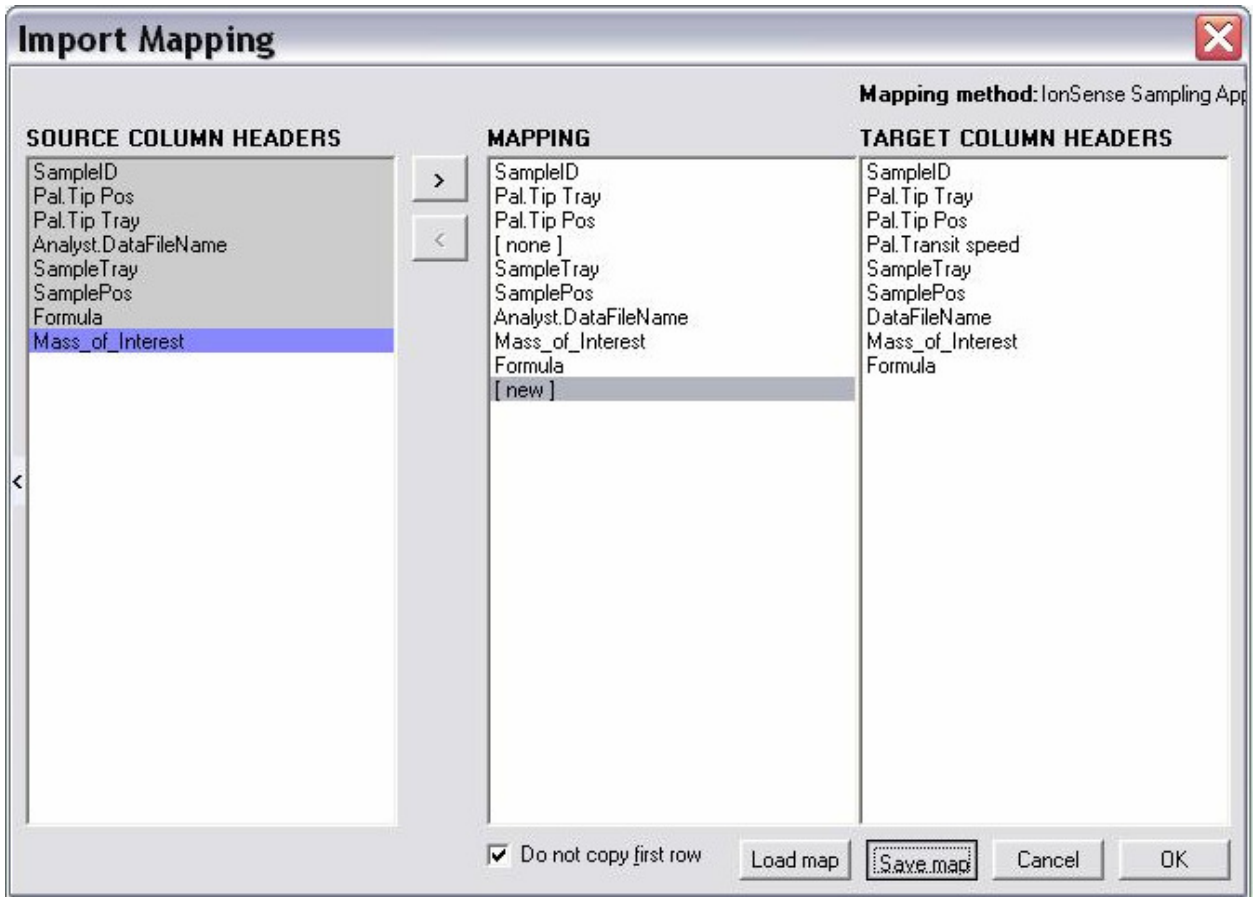


For the “Reference” select “Analyst” from the drop down box. Click “Ok” to save the changes and create the “Formula” column header in the LEAP Shell “Target Column Headers”.





When all of the “Source Column Headers” have been mapped to one of the LEAP Shell “Target Column Headers” select “**Save map**” at the bottom of the window to save a copy of the map for future use. To complete the mapping without saving the map, select “Ok”.



By selecting “**Save map**” a “Save As” window will appear where the map can be named and saved to a safe location.

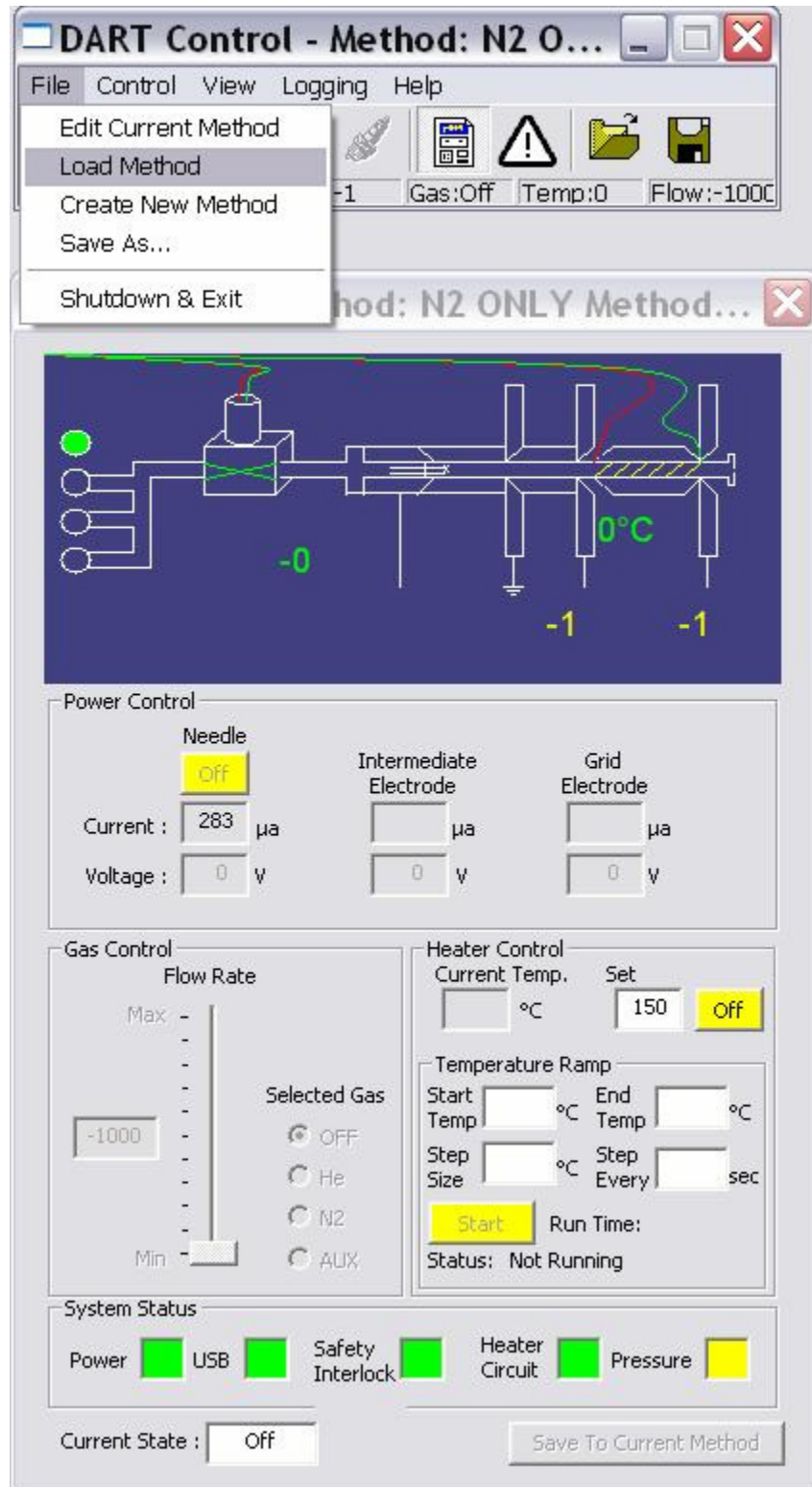
After saving the mapping file or proceeding without saving the mapping file, the LEAP Shell sample list view will appear as shown below. LEAP Shell will prompt the user to name the sample list and save it under “Sample Lists” within LEAP Shell.

The screenshot displays the LEAP Shell - PAL and Analyst software interface. The main window shows a table of sample lists with columns for SampleID, Shell Method, Pal.Tip Tray, Pal.Tip Pos, Pal.Transit speed, SampleTray, SamplePos, DataFileName, Mass\_of\_I..., and Formula. A dialog box titled "Sample list" is open, prompting the user to save the list with the name "DART Samples IMPORTED SAMPLE LIST".

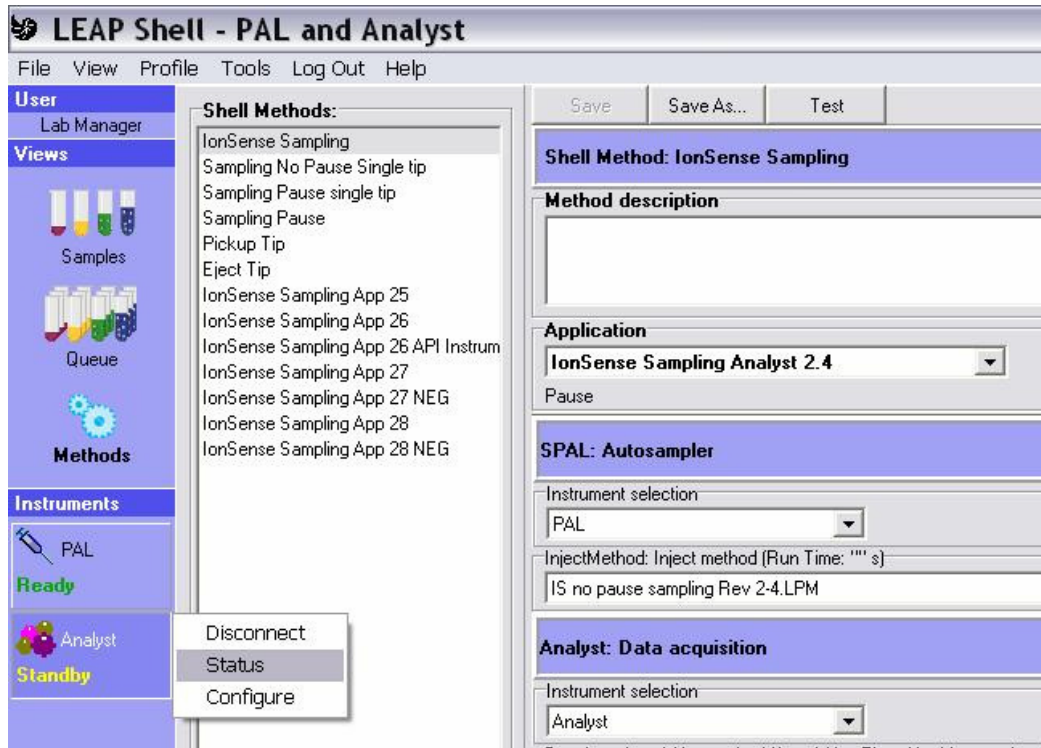
SampleID	Shell Method	Pal.Tip Tray	Pal.Tip Pos	Pal.Transit speed	SampleTray	SamplePos	DataFileName	Mass_of_I...	Formula	
1	Analyst Sample Name 1	IonSense Sam...	Tip-01	1	500	Sample01	1	Analyst WIFF File Name_001	206.04	C7H6BF3O3
2	Analyst Sample Name 2	IonSense Sam...	Tip-01	2	500	Sample01	2	Analyst WIFF File Name_002	206.04	C7H6BF3O3
3	Analyst Sample Name 3	IonSense Sam...	Tip-01	3	500	Sample01	3	Analyst WIFF File Name_003	206.04	C7H6BF3O3
4	Analyst Sample Name 4	IonSense Sam...	Tip-01	4	500	Sample01	4	Analyst WIFF File Name_004	206.04	C7H6BF3O3
5	Analyst Sample Name 5	IonSense Sam...	Tip-01	5	500	Sample01	5	Analyst WIFF File Name_005	206.04	C7H6BF3O3
6	Analyst Sample Name 6	IonSense Sam...	Tip-01	6	500	Sample01	6	Analyst WIFF File Name_006	206.04	C7H6BF3O3
7	Analyst Sample Name 7	IonSense Sam...	Tip-01	7	500	Sample01	7	Analyst WIFF File Name_007	206.04	C7H6BF3O3
8	Analyst Sample Name 8	IonSense Sam...	Tip-01	8	500	Sample01	8	Analyst WIFF File Name_008	206.04	C7H6BF3O3
9	Analyst Sample Name 9	IonSense Sam...	Tip-01	9	500	Sample01	9	Analyst WIFF File Name_009	206.04	C7H6BF3O3
10	Analyst Sample Name 10	IonSense Sam...	Tip-01	10	500	Sample01	10	Analyst WIFF File Name_010	206.04	C7H6BF3O3
11	Analyst Sample Name 11	IonSense Sam...	Tip-01	11	500	Sample01	11	Analyst WIFF File Name_011	206.04	C7H6BF3O3
12	Analyst Sample Name 12	IonSense Sam...	Tip-01	12	500	Sample01	12	Analyst WIFF File Name_012	206.04	C7H6BF3O3
13	Analyst Sample Name 13	IonSense Sam...	Tip-01	13	500	Sample01	13	Analyst WIFF File Name_013	206.04	C7H6BF3O3
14	Analyst Sample Name 14	IonSense Sam...	Tip-01	14	500	Sample01	14	Analyst WIFF File Name_014	206.04	C7H6BF3O3
15	Analyst Sample Name 15	IonSense Sam...	Tip-01	15	500	Sample01	15	Analyst WIFF File Name_015	206.04	C7H6BF3O3
16	Analyst Sample Name 16	IonSense Sam...	Tip-01	16	500	Sample01	16	Analyst WIFF File Name_016	206.04	C7H6BF3O3
17	Analyst Sample Name 17	IonSense Sam...	Tip-01	17	500	Sample01	17	Analyst WIFF File Name_017	206.04	C7H6BF3O3
18	Analyst Sample Name 18	IonSense Sam...	Tip-01	18	500	Sample01	18	Analyst WIFF File Name_018	206.04	C7H6BF3O3
19	Analyst Sample Name 19	IonSense Sam...	Tip-01	19	500	Sample01	19	Analyst WIFF File Name_019	206.04	C7H6BF3O3
20	Analyst Sample Name 20	IonSense Sam...	Tip-01	20	500	Sample01	20	Analyst WIFF File Name_020	206.04	C7H6BF3O3
21	Analyst Sample Name 21	IonSense Sam...	Tip-01	21	500	Sample01	21	Analyst WIFF File Name_021	206.04	C7H6BF3O3
22	Analyst Sample Name 22	IonSense Sam...	Tip-01	22	500	Sample01	22	Analyst WIFF File Name_022	206.04	C7H6BF3O3
23	Analyst Sample Name 23	IonSense Sam...	Tip-01	23	500	Sample01	23	Analyst WIFF File Name_023	206.04	C7H6BF3O3
24	Analyst Sample Name 24	IonSense Sam...	Tip-01	24	500	Sample01	24	Analyst WIFF File Name_024	206.04	C7H6BF3O3
25	Analyst Sample Name 25	IonSense Sam...	Tip-01	25	500	Sample01	25	Analyst WIFF File Name_025	206.04	C7H6BF3O3
26	Analyst Sample Name 26	IonSense Sam...	Tip-01	26	500	Sample01	26	Analyst WIFF File Name_026	206.04	C7H6BF3O3
27	Analyst Sample Name 27	IonSense Sam...	Tip-01	27	500	Sample01	27	Analyst WIFF File Name_027	206.04	C7H6BF3O3
28	Analyst Sample Name 28	IonSense Sam...	Tip-01	28	500	Sample01	28	Analyst WIFF File Name_028	206.04	C7H6BF3O3
29	Analyst Sample Name 29	IonSense Sam...	Tip-01	29	500	Sample01	29	Analyst WIFF File Name_029	206.04	C7H6BF3O3
30	Analyst Sample Name 30	IonSense Sam...	Tip-01	30	500	Sample01	30	Analyst WIFF File Name_030	206.04	C7H6BF3O3
31	Analyst Sample Name 31	IonSense Sam...	Tip-01	31	500	Sample01	31	Analyst WIFF File Name_031	206.04	C7H6BF3O3
32	Analyst Sample Name 32	IonSense Sam...	Tip-01	32	500	Sample01	32	Analyst WIFF File Name_032	206.04	C7H6BF3O3
33	Analyst Sample Name 33	IonSense Sam...	Tip-01	33	500	Sample01	33	Analyst WIFF File Name_033	206.04	C7H6BF3O3
34	Analyst Sample Name 34	IonSense Sam...	Tip-01	34	500	Sample01	34	Analyst WIFF File Name_034	206.04	C7H6BF3O3
35	Analyst Sample Name 35	IonSense Sam...	Tip-01	35	500	Sample01	35	Analyst WIFF File Name_035	206.04	C7H6BF3O3
36	Analyst Sample Name 36	IonSense Sam...	Tip-01	36	500	Sample01	36	Analyst WIFF File Name_036	206.04	C7H6BF3O3
37	Analyst Sample Name 37	IonSense Sam...	Tip-01	37	500	Sample01	37	Analyst WIFF File Name_037	206.04	C7H6BF3O3
38	Analyst Sample Name 38	IonSense Sam...	Tip-01	38	500	Sample01	38	Analyst WIFF File Name_038	206.04	C7H6BF3O3
39	Analyst Sample Name 39	IonSense Sam...	Tip-01	39	500	Sample01	39	Analyst WIFF File Name_039	206.04	C7H6BF3O3
40	Analyst Sample Name 40	IonSense Sam...	Tip-01	40	500	Sample01	40	Analyst WIFF File Name_040	206.04	C7H6BF3O3

## Getting Ready to Run

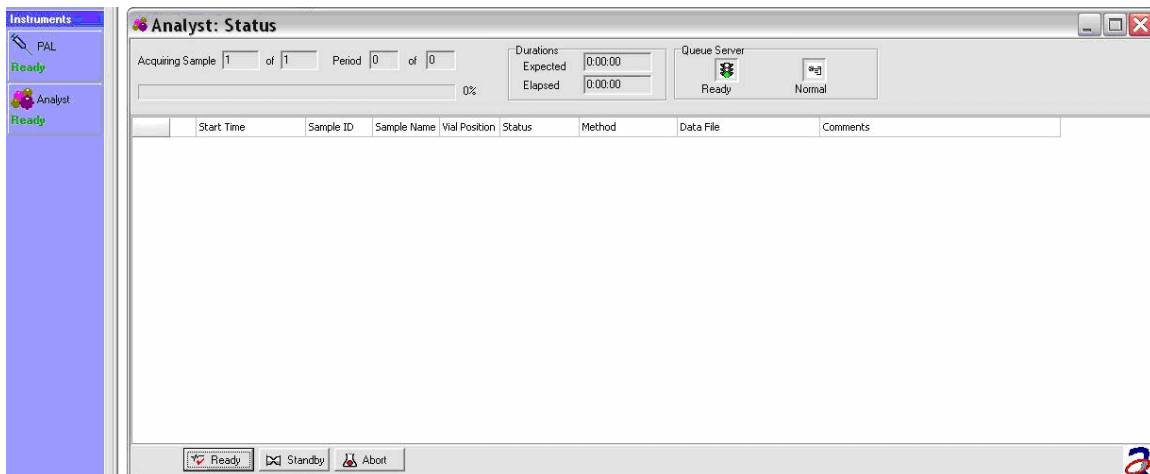
To prepare to run make sure that the **DART Control software** has been **opened** and the desired **DART Method** has been **loaded**.



In LEAP Shell, check that all “**Instruments**” are in the “**Ready**” mode. When connecting to Analyst through LEAP Shell the default Analyst mode will be “**Standby**”, the user can “**Ready**” Analyst through the “Analyst: Status” window.



In the “Analyst: Status” window click on “**Ready**” to put Analyst in the “**Ready**” mode.





## Submit the Sample List to the LEAP Shell Queue and Run

View of the LEAP Shell Sample Queue.

The screenshot shows the LEAP Shell - PAL and Analyst window. The main area displays a table titled "DART Samples IMPORTED SAMPLE LIST". The table has columns for Time Stamp, Status, SampleID, Shell Method, Pal.Tip Tray, Pal.Tip Pos, Pal.Transit speed, SampleTray, SamplePos, DataFileName, Mass\_of\_In..., and Formula. The first row is highlighted in green, indicating it is running.

	Time Stamp	Status	SampleID	Shell Method	Pal.Tip Tray	Pal.Tip Pos	Pal.Transit speed	SampleTray	SamplePos	DataFileName	Mass_of_In...	Formula
1	12/26/2008 10:24:07...	Running	Analyst Sample Name 1	IonSense Samplin...	Tip-01	1	500	Sample01	1	Analyst WIFF File Name_001	206.04	C7H6BF303
2	10:23:50 AM	Waiting	Analyst Sample Name 2	IonSense Samplin...	Tip-01	2	500	Sample01	2	Analyst WIFF File Name_002	206.04	C7H6BF303
3	10:23:50 AM	Waiting	Analyst Sample Name 3	IonSense Samplin...	Tip-01	3	500	Sample01	3	Analyst WIFF File Name_003	206.04	C7H6BF303
4	10:23:50 AM	Waiting	Analyst Sample Name 4	IonSense Samplin...	Tip-01	4	500	Sample01	4	Analyst WIFF File Name_004	206.04	C7H6BF303
5	10:23:50 AM	Waiting	Analyst Sample Name 5	IonSense Samplin...	Tip-01	5	500	Sample01	5	Analyst WIFF File Name_005	206.04	C7H6BF303
6	10:23:50 AM	Waiting	Analyst Sample Name 6	IonSense Samplin...	Tip-01	6	500	Sample01	6	Analyst WIFF File Name_006	206.04	C7H6BF303
7	10:23:50 AM	Waiting	Analyst Sample Name 7	IonSense Samplin...	Tip-01	7	500	Sample01	7	Analyst WIFF File Name_007	206.04	C7H6BF303
8	10:23:50 AM	Waiting	Analyst Sample Name 8	IonSense Samplin...	Tip-01	8	500	Sample01	8	Analyst WIFF File Name_008	206.04	C7H6BF303
9	10:23:50 AM	Waiting	Analyst Sample Name 9	IonSense Samplin...	Tip-01	9	500	Sample01	9	Analyst WIFF File Name_009	206.04	C7H6BF303
10	10:23:50 AM	Waiting	Analyst Sample Name 10	IonSense Samplin...	Tip-01	10	500	Sample01	10	Analyst WIFF File Name_010	206.04	C7H6BF303
11	10:23:50 AM	Waiting	Analyst Sample Name 11	IonSense Samplin...	Tip-01	11	500	Sample01	11	Analyst WIFF File Name_011	206.04	C7H6BF303
12	10:23:50 AM	Waiting	Analyst Sample Name 12	IonSense Samplin...	Tip-01	12	500	Sample01	12	Analyst WIFF File Name_012	206.04	C7H6BF303
13	10:23:50 AM	Waiting	Analyst Sample Name 13	IonSense Samplin...	Tip-01	13	500	Sample01	13	Analyst WIFF File Name_013	206.04	C7H6BF303
14	10:23:50 AM	Waiting	Analyst Sample Name 14	IonSense Samplin...	Tip-01	14	500	Sample01	14	Analyst WIFF File Name_014	206.04	C7H6BF303
15	10:23:50 AM	Waiting	Analyst Sample Name 15	IonSense Samplin...	Tip-01	15	500	Sample01	15	Analyst WIFF File Name_015	206.04	C7H6BF303

At the bottom of the LEAP Shell window the “DART Warm-up Time” set through the LEAP Shell Method will be displayed. The time posted in the message is the time that the PAL will begin running the samples in the Queue. This example shows a 5 minute “DART Warm-up Time”.

```
[13:02:21 ]>>
[13:02:21 ]>> === RUNNING SAMPLE LIST ===
[13:02:21 ]>> Waiting for DART To Warm up - Ready at 1:07:21 PM
[13:03:46 ]>>
```

The status of the Analyst data acquisition can be checked through LEAP Shell by accessing the “Analyst: Status” window. Left click on the “Analyst” icon under “Instruments” and select “Status” to open the “Analyst: Status” window shown below.

The screenshot shows the Analyst: Status window. At the top, it displays "Acquiring Sample 1 of 1" and "Period 1 of 1". Below this is a progress bar showing 55% completion. To the right, there are fields for "Durations Expected" (0:00:20) and "Elapsed" (0:00:11). Further right, there are "Queue Server" options: "Acquiring" (selected) and "Normal".

	Start Time	Sample ID	Sample Name	Vial Position	Status	Method	Data File	Comments
1	12/26/2008 10:24:25 F	Analyst Samp	Analyst Samp	1	Acquired	Sciex Test Meth	Analyst WIFF File Name_001	
2	12/26/2008 10:25:25 F	Analyst Samp	Analyst Samp	2	Acquired	Sciex Test Meth	Analyst WIFF File Name_002	
3	12/26/2008 10:26:16 F	Analyst Samp	Analyst Samp	3	Acquired	Sciex Test Meth	Analyst WIFF File Name_003	
4	12/26/2008 10:27:07 F	Analyst Samp	Analyst Samp	4	Acquired	Sciex Test Meth	Analyst WIFF File Name_004	
5	12/26/2008 10:28:00 F	Analyst Samp	Analyst Samp	5	Acquired	Sciex Test Meth	Analyst WIFF File Name_005	
6	12/26/2008 10:28:52 F	Analyst Samp	Analyst Samp	6	Acquired	Sciex Test Meth	Analyst WIFF File Name_006	
7	12/26/2008 10:29:43 F	Analyst Samp	Analyst Samp	7	Acquired	Sciex Test Meth	Analyst WIFF File Name_007	
8	12/26/2008 10:30:34 F	Analyst Samp	Analyst Samp	8	Acquired	Sciex Test Meth	Analyst WIFF File Name_008	
9	12/26/2008 10:31:38 F	Analyst Samp	Analyst Samp	9	Acquired	Sciex Test Meth	Analyst WIFF File Name_009	
10	12/26/2008 10:32:29 F	Analyst Samp	Analyst Samp	10	Acquiring	Sciex Test Meth	Analyst WIFF File Name_010	

## ***DART Shutdown Feature***

At the end of any submitted batch in the LEAP Shell Sample Queue DART Control is triggered by LEAP Shell to shutdown.

- **DART Control** is placed into “**Standby**” mode with the heater “**ON**”.
- The **DART heater** will be turned **off in 3 minutes** after being placed in “Standby” by the DART Shutdown feature.
- **DART Control** will be completely turned “**OFF**” in a total of 5 minutes.

In the event that:

- There are multiple sample batches in the queue, the DART will not be shut down until the last sample batch submitted has finished running. Note: If a “DART Warm-up Time” has been set in the LEAP Shell Method it will be executed at the beginning of every sample batch.
  - It is suggested that for multiple sample batch submissions to not include a “DART Warm-up Time” in the LEAP Shell Method. For this case it is advised to allow the DART to fully heat in “Standby” before starting the run through LEAP Shell. LEAP Shell will automatically turn DART Control into “Run” mode.
- The user wishes to cancel the DART Shutdown at any time click the “**Cancel**” button in the “DART Shutdown” window.

View of the DART Shutdown window at the end of a LEAP Shell run.



## ***Additional Comments***

By design, many of the user configurable features in the automated version of the MSRedux-XI software can only be set by the interactive (GUI) version and are inaccessible from LEAP Shell.