

Using a Script to Load a Set of Experimental Raw Data into a Project

ACD/Method Development Suite AutoChrom Console
Version 10.01

Irina Oshchepkova and Andrey Vazhentsev
Advanced Chemistry Development, Inc.
Toronto, ON, Canada
www.acdlabs.com

Introduction

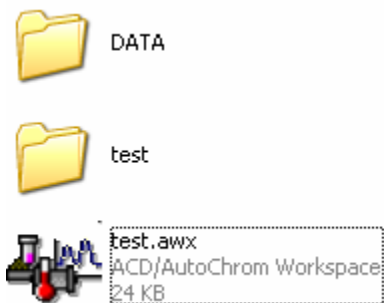
This Technical Note will describe how to install, configure, and use a script to automate the process of loading the raw data files into an ACD/Method Development Suite^{1,2} (MDS) project created for the "Virtual Instrument". This script is useful tool since it allows you to import all the experimental data at once and place them to the appropriate Wave. This is especially useful for situations where many injections were performed at once, and there are several data files to import into the AutoChrom Console.

The script requires ACD/Method Development Suite (for LC/MS or LC/UV) version 10.01 or higher. We will operate in the AutoChrom Console.

Prepare the Files

Before using the script, you need to create a project and place all the raw data files in one place. For this example, the EXAMPLE.ZIP file will be utilized.

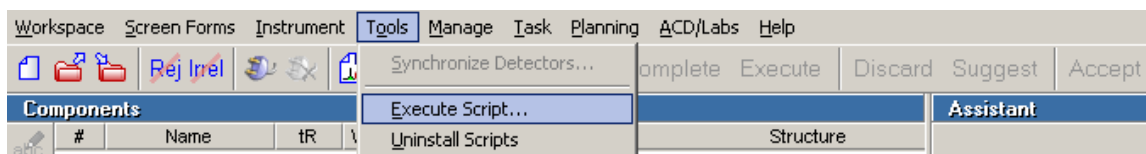
1. Download the EXAMPLE.ZIP file from our web site at http://www.acdlabs.com/download/technotes/100/chrom/mds_example.zip and save it to your computer.
2. Extract all the files and folders contained in the EXAMPLE.ZIP.
3. As a result, you will see three extracted objects: a project that contains a TEST.AWX file, a folder with the same name (test), and the DATA folder containing the raw data files that will be eventually attached to the project and the RAWDATA_BINDING.INI file that will be used by the script.



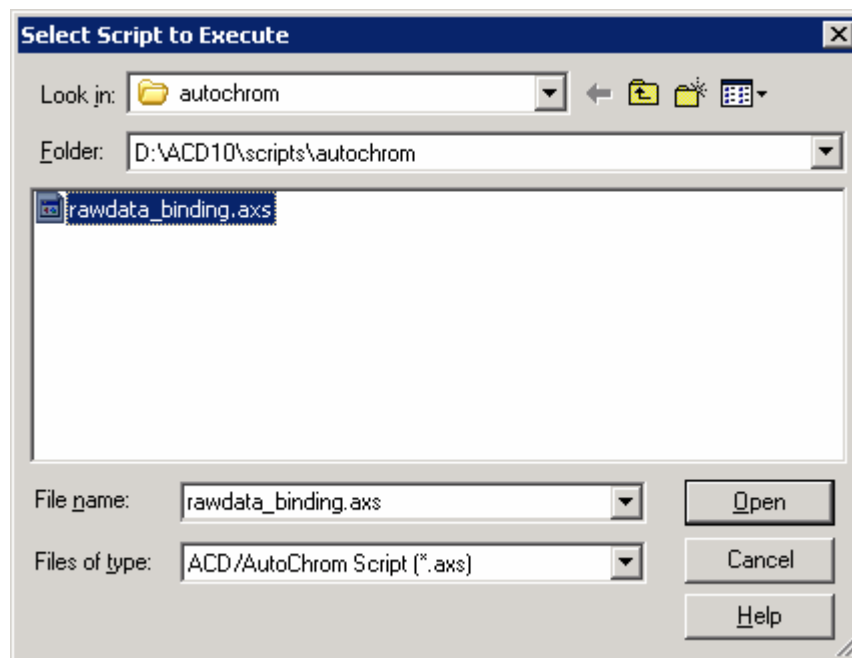
Note Please note that all the raw data files need to be stored in the same folder and be named in the same manner.

Install the Script

1. Download the RAWDATA_BINDING.ZIP file from our web site at http://www.acdlabs.com/download/technotes/100/chrom/mds_rawdata_binding.zip and save it to the ACD10\SCRIPTS\AUTOCHROM directory.
2. Extract the RAWDATA_BINDING.AXS file to the same folder.
3. Open the ACD/Method Development Suite AutoChrom Console. From the Windows **Start** menu, select **All Programs**. Select **ACDLABS 10** from the list of programs, and choose **AutoChrom**.
4. With the AutoChrom Console running, in the Task or Workspace window, from the **Tools** menu, choose **Execute Script**.



5. In the **Select Script to Execute** dialog box that appears, navigate to the RAWDATA_BINDING.AXS file and click **Open**.



6. The script has now been installed, although you will not receive a confirmation message.

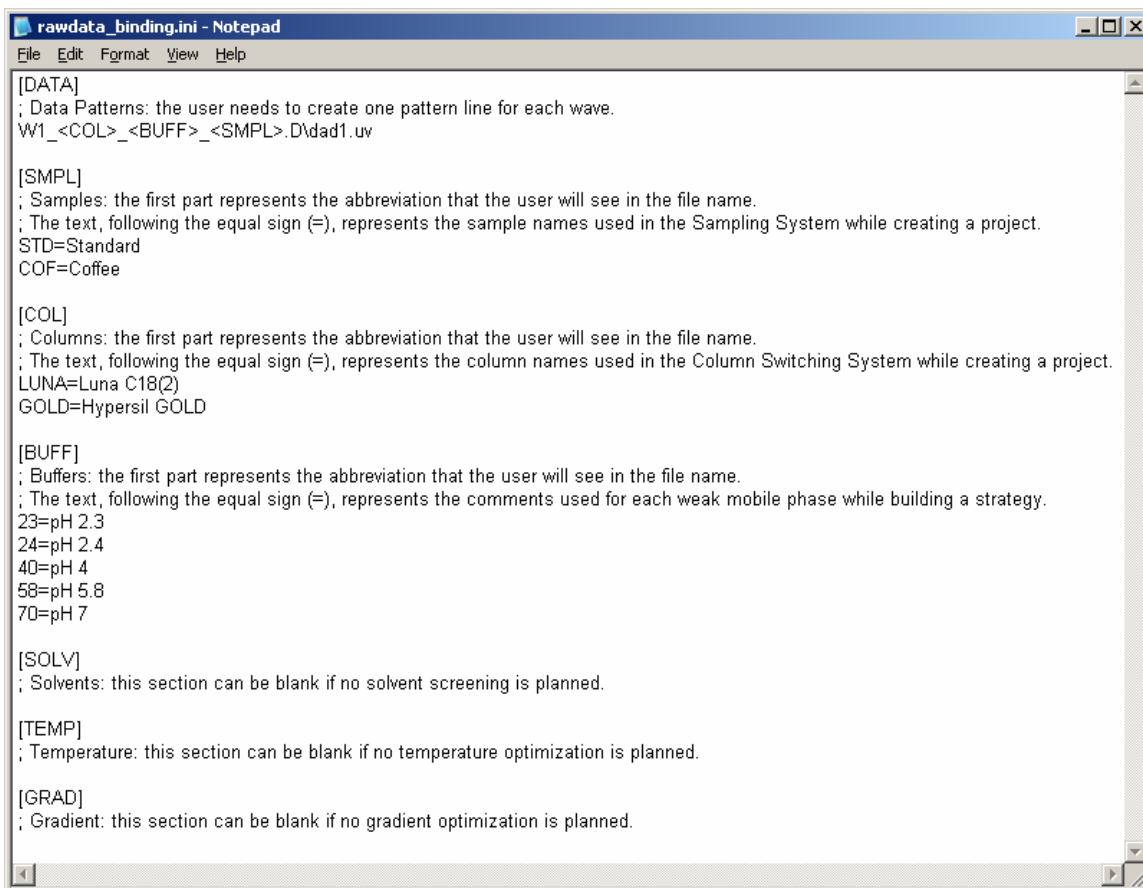
Note You may notice that when you run the script, you are prompted with the same windows a few times. This indicates that the script was installed more than once. To avoid repetition, uninstall the scripts first and then install the required one again. In the latest version of the AutoChrom Console, you will be able to control that and activate the desired script when starting the program.

Prepare the Configuration *.INI File

Chromatograms in MDS projects are arranged according to chromatographic method and sample identifier. The script we are going to use needs to recognize the raw data files by their names and attach them to the appropriate place in the project. To do that properly, this script uses the contents of the special configuration file.

For this example, the RAWDATA_BINDING.INI file will be used. This file is included in the DATA folder where we stored all the raw data files.

You can open the RAWDATA_BINDING.INI file in Notepad to see its contents.



```
rawdata_binding.ini - Notepad
File Edit Format View Help
[DATA]
; Data Patterns: the user needs to create one pattern line for each wave.
W1_<COL>_<BUFF>_<SMPL>.D\dad1.uv

[SMPL]
; Samples: the first part represents the abbreviation that the user will see in the file name.
; The text, following the equal sign (=), represents the sample names used in the Sampling System while creating a project.
STD=Standard
COF=Coffee

[COL]
; Columns: the first part represents the abbreviation that the user will see in the file name.
; The text, following the equal sign (=), represents the column names used in the Column Switching System while creating a project.
LUNA=Luna C18(2)
GOLD=Hypersil GOLD

[BUFF]
; Buffers: the first part represents the abbreviation that the user will see in the file name.
; The text, following the equal sign (=), represents the comments used for each weak mobile phase while building a strategy.
23=pH 2.3
24=pH 2.4
40=pH 4
58=pH 5.8
70=pH 7

[SOLV]
; Solvents: this section can be blank if no solvent screening is planned.

[TEMP]
; Temperature: this section can be blank if no temperature optimization is planned.

[GRAD]
; Gradient: this section can be blank if no gradient optimization is planned.
```

If you have more than one project, it is recommended to create one configuration file per project and keep it inside the folder where the raw data are stored. In this case, the script will apply different rules for different data. If you deal with the same data type and keep the data names constant, it is possible to create one generic *.INI file and place it in the ACD10\SCRIPTS\AUTOCHROM folder. The script will check for the configuration file in the folder with the raw data first and if it cannot find it, the generic *.INI file will be used.

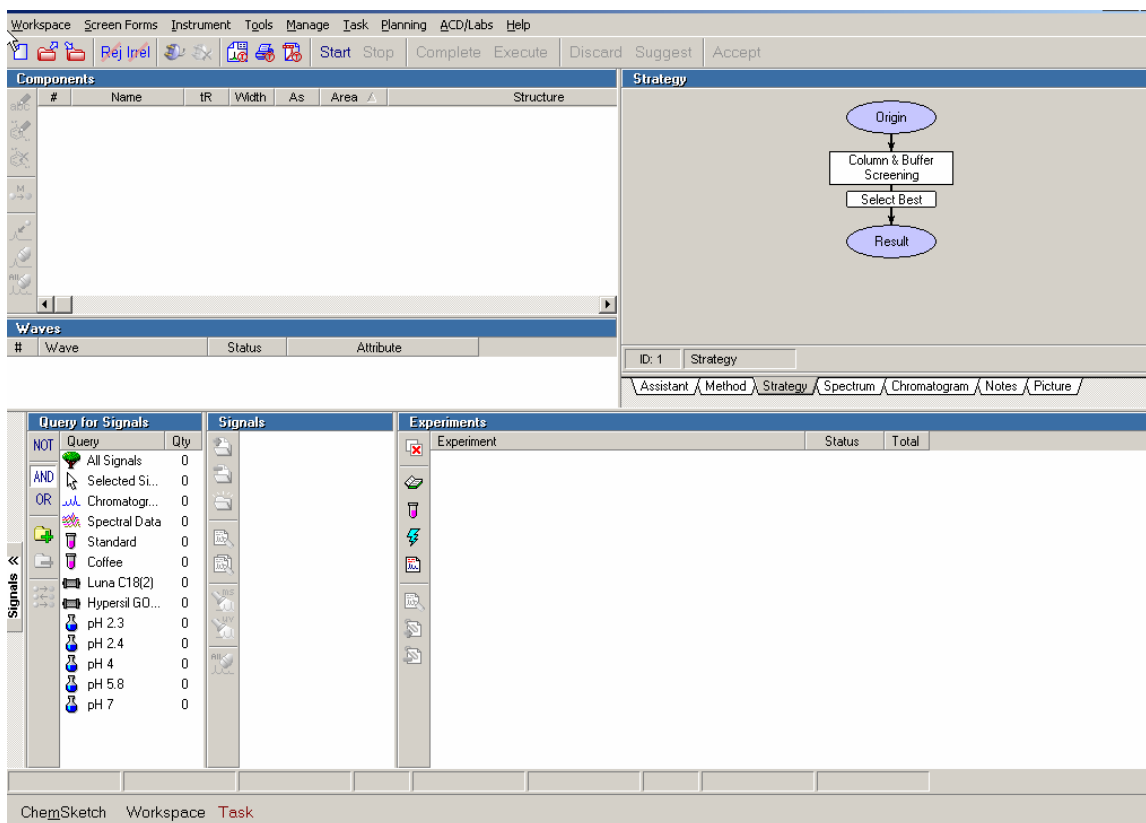
For more details on how to create a configuration file, refer to *Appendix A* below.

Execute the Script

When working with the project, you perform the following main steps: creating a project, building a strategy, and executing the planned injections. For the Virtual Instrument, you need to bring in each experimental data file manually one by one. The script allows you to avoid this process by attaching all the raw data related to the project wave in a single step.

We will be working with the TEST.AWX project that was previously downloaded and extracted.

1. Open the TEST.AWX file.



The screenshot displays the ChemSketch software interface with the following components:

- Menu Bar:** Workspace, Screen Forms, Instrument, Tools, Manage, Task, Planning, ACD/Labs, Help.
- Toolbar:** Rej Inel, Start, Stop, Complete, Execute, Discard, Suggest, Accept.
- Components Table:**

#	Name	IR	Width	As	Area	Structure
- Strategy Diagram:**

```

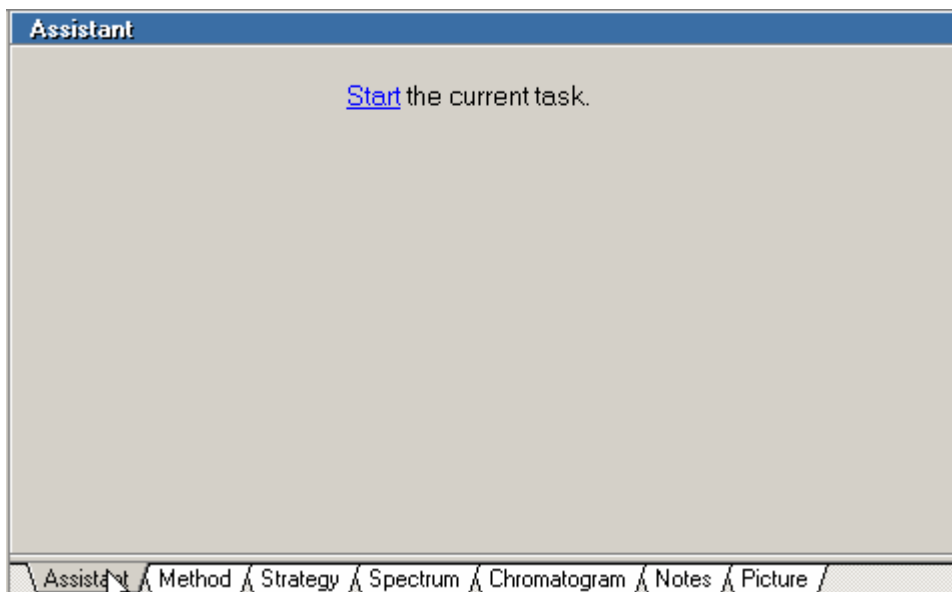
graph TD
    Origin([Origin]) --> Screening[Column & Buffer Screening]
    Screening --> SelectBest[Select Best]
    SelectBest --> Result([Result])
    
```
- Waves Table:**

#	Wave	Status	Attribute
- Query for Signals Table:**

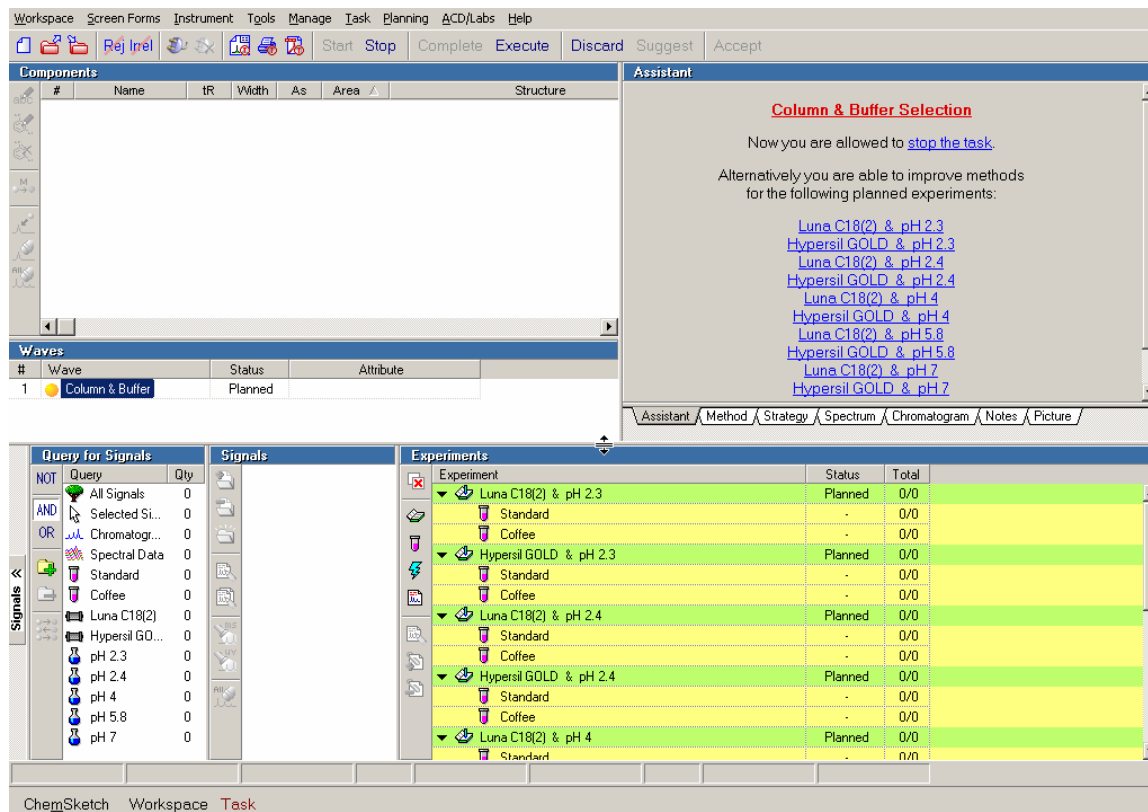
Query	Qty
All Signals	0
Selected Si...	0
Chromatogr...	0
Spectral Data	0
Standard	0
Coffee	0
Luna C18(2)	0
Hypersil G0...	0
pH 2.3	0
pH 2.4	0
pH 4	0
pH 5.8	0
pH 7	0
- Experiments Table:**

Experiment	Status	Total
- Bottom Bar:** ChemSketch Workspace Task

- Switch to the **Assistant** tab and click the **Start** link.



- You will see all the possible methods listed. You will need to provide data for each method.



The screenshot shows the ChemSketch workspace with the Assistant window open. The Assistant window displays a 'Column & Buffer Selection' dialog. The main workspace shows a 'Waves' table with one entry: 'Column & Buffer' (Planned). Below the Assistant window, there are three panels: 'Query for Signals', 'Signals', and 'Experiments'.

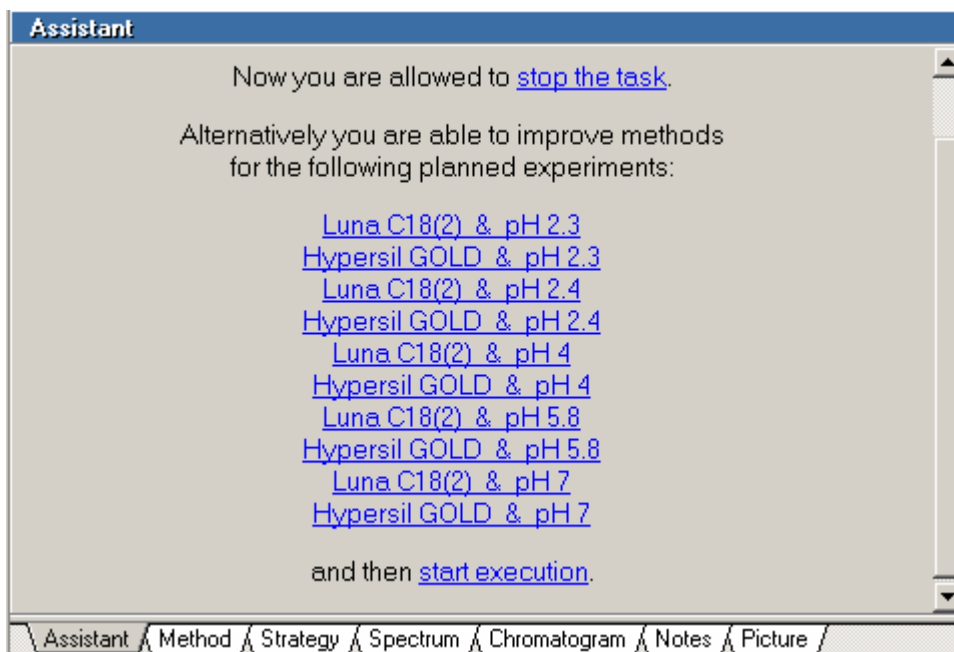
#	Wave	Status	Attribute
1	Column & Buffer	Planned	

Query	Qty
All Signals	0
Selected Si...	0
Chromatogr...	0
Spectral Data	0
Standard	0
Coffee	0
Luna C18(2)	0
Hypersil GO...	0
pH 2.3	0
pH 2.4	0
pH 4	0
pH 5.8	0
pH 7	0

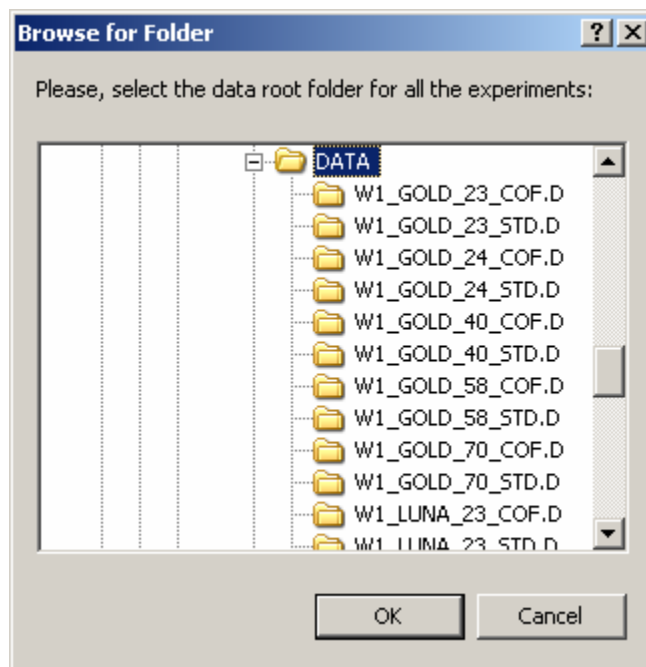
Experiment	Status	Total
Luna C18(2) & pH 2.3	Planned	0/0
Standard	-	0/0
Coffee	-	0/0
Hypersil GOLD & pH 2.3	Planned	0/0
Standard	-	0/0
Coffee	-	0/0
Luna C18(2) & pH 2.4	Planned	0/0
Standard	-	0/0
Coffee	-	0/0
Hypersil GOLD & pH 2.4	Planned	0/0
Standard	-	0/0
Coffee	-	0/0
Luna C18(2) & pH 4	Planned	0/0
Standard	-	0/0

ChemSketch Workspace Task

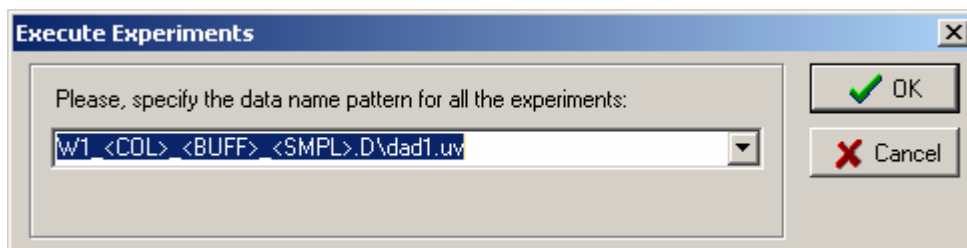
4. Scroll down in the **Assistant** tab and click the *start execution* link.



5. The **Browse for Folder** dialog box appears where you can specify the root folder containing all the raw data and then click **OK**.



6. The script is communicating with the RAWDATA_BINDING.INI configuration file and the **Execute Experiments** dialog box appears. You can see the suggested data filename pattern that will be used for all experiments. If the project includes more than one wave, clicking the drop-down box will show all the available patterns. You may select any item from the drop-down box or type in a new pattern manually.



7. By clicking **OK**, you have accepted the chosen pattern and the script starts executing.
8. The script is creating the full pathname to the raw data file for each planned injection, and at the same time it checks if each file exists in the specified directory.

Note When the pathname for an injection cannot be constructed, an error message will appear. This error message may arise if there is not enough information in the configuration file or the file does not exist. When the error appears, the script starts working from the beginning.

Experiments			
Experiment	Status	Total	
▼ Luna C18(2) & pH 2.3	Complete	0/0	
▼ Standard	-	0/0	
▼ Trial #1	Complete	0/0	
UV dad1.uv	Complete	0/0	
UV dad1A.ch	Complete	0/0	
▼ Coffee	-	0/0	
▼ Trial #1	Complete	0/0	
UV dad1.uv	Complete	0/0	
UV dad1A.ch	Complete	0/0	
▼ Hypersil GOLD & pH 2.3	Complete	0/0	
▼ Standard	-	0/0	
▼ Trial #1	Complete	0/0	
UV dad1.uv	Complete	0/0	
UV dad1A.ch	Complete	0/0	

Uninstall the Script

In the **Task** or **Workspace** window, from the **Tools** menu, choose **Uninstall Scripts**. It allows you to uninstall all the scripts that were previously installed.

Note Currently, in version 10.01, you cannot uninstall the scripts separately.

Appendix A: Examples

The *data name pattern* is a conventional string which represents the portion of the pathname to each raw data file, following after the *data root folder*. For example, if the *data root folder* is D:\DATA, and the *data name pattern* is EXP<COL>\MSD1.MS, then the full path name to each raw data file will be D:\DATA\ EXP<COL>\MSD1.MS, where <COL> means column name and will be replaced by a certain substring, depending on the column used in the method for each planned experiment. This information is specified in the configuration INI file. Please note that in addition to MSD1.MS file, the *.CH and *.UV files from the same folder will be appended to the injection. It is a very convenient approach when all logically connected data are automatically appended at once.

When dealing with MassLynx data, the data name pattern should specify the path to the _FUNCTNS.INF file inside the *.RAW folder.

Note It is possible to click **Cancel** in almost every dialog box. In this case, the execution of the script is interrupted and you are prompted to execute the experiments in the regular way.

Appendix B: Contents of the *.INI File

Before executing all the planned experiments, you should prepare the RAWDATA_BINDING.INI configuration file and place it in the folder where all the raw data files are located. If you are going to use the same configuration file for all the Waves and Tasks, then it is recommended to put this default configuration file into ACD/Labs installation folder:

<ACD-FOLDER>\SCRIPTS\AUTOCHROM\

The configuration file is a text file that can be created in any text editor, such as Notepad. The file contains several standard sections:

```
[DATA]
Pattern1
Pattern2
.....
PatternN
```

In this section, all the known “*data name patterns*” are specified. The list of strings from this section will be used in the **Execute Experiments** dialog box (i.e., **Step 2**). Usually, you will have at least one pattern for each Wave, because the *naming rules* depend on the variable parameters in the Wave.

Here are some examples of the “wildcards” used in the *data name patterns* that will be eventually replaced by certain substring from the particular injection:

- <COL> method column
- <SOLV> method strong phase, solvent
- <BUFF> method weak phase, buffer
- <GRAD> method gradient program
- <TEMP> method temperature
- <SMPL> injection sample

The substrings that will be used to replace each “wildcard” for specific injection are specified in the corresponding sections of the configuration file:

[COL], [SOLV], [BUFF], [GRAD], [TEMP], [SMPL].

The order of the sections is not important and sections can be skipped. In each of these sections, you should specify a list of **substitution rules**. Each rule looks like this:

Replacement_Substring = Parameter_value

For example, the rule **COL1=Xbridge C18** in the section **[COL]** means that for every injection with method column Xbridge C18, the “wildcard” **<COL>** in the *data name pattern* should be replaced with substring “COL1”. The number of rules in each section is not limited; you may have several rules with the same “Replacement_substring”.

The “Parameter_value” is a string that represents the value of the parameter in the **corresponding section**:

For the **[COL]** section, this is just the name of the column used in the method without specifying the column parameters; such as length or diameter, only name of the column as it is specified in the Workspace.

For the **[SOLV]** section, this is a textual representation of the strong phase (solvent). You can observe this text in the status bar when the corresponding experiment is selected. For Tasks that perform Solvent Screening, instead of textual representation of the strong phase, the value of “**Comment**” for the strong phase will be used. You can also use any unique strings in the “**Comment**” for strong phase and all of these strings can be used as “Parameter_value” for any rule in the considered section.

For the **[BUFF]** section, this is a textual representation of the method weak phase (buffer). The text will appear in the status bar when the corresponding experiment is selected. For Tasks that perform Buffer Screening, instead of textual representation of the weak phase, the value of “**Comment**” for this weak phase will be used.

For the **[GRAD]** section, this is a textual representation of the method gradient program. You can see this text in the status bar and in many other places in the program. Here are some examples of the gradient program: **50%, 0–80% (16 min)** and **0–50% (12 min); 50–80% (7 min)**. The space in these strings is very important. You should not input these strings manually. It can be copied from the Task window (for example, by clicking on the corresponding panel of the status bar) and then pasted to the configuration file. The same approach can be applied for specifying any other parameters, such as Column, Solvent, Buffer, Temperature, or Sample.

For the **[TEMP]** section, this is a textual representation of the method temperature such as **35°C** or **60°C**.

Note The degree symbols are very important in these strings, and spaces in the middle are not allowed. It is better to be copied from the status bar.

For the **[SMPL]** section, this is a name of the corresponding injection **Probe** (usually it is equal to the name of the Sample, but you can change the name of the Probe to any other value at any time). You can also take this information from the status bar.

Conclusion

Systematic data import using this script can save a great deal of time and allows you to input the experimental data files faster and more accurately. This is particularly useful when chromatographers consistently apply similar strategies to their method development tasks.

References

1. ACD/Method Development Suite for LC/MS. www.acdlabs.com/meth_develop/ Advanced Chemistry Development, Inc., Toronto, ON, Canada. 17 April 2007.
2. ACD/Method Development Suite for LC/UV. www.acdlabs.com/mds_lcu/ Advanced Chemistry Development, Inc., Toronto, ON, Canada. 17 April 2007.