PAL Cycle Composer and Drivers

Installation Guide
User Manual
Software Revision 1.5.4

Printing History

Edition 1	September 1998	Software Revision CC1.0
Edition 2	July 1999	Software Revision CC1.3
Edition 3	November 1999	Software Revision CC1.4
Edition 4	October 2000	Manual including Drivers (combined Manual, no change in Software Revision
Edition 5	May 2001	Software Revision CC1.5 Agilent ChemStation Driver Revision 2.0.3 ThermoFinnigan Xcalibur Driver Revision 1.3
Edition 6	June 2001	Software Revision CC 1.5 Agilent ChemStation Driver Revision 2.0.4 ThermoFinnigan Xcalibur Driver Revision 1.3
Edition 7	July 2001	Software Revision CC 1.5 Agilent ChemStation Driver 2.0.4 ThermoFinnigan Driver 1.3.1
Edition 8	May 2007	Software Revision CC 1.5.4 Agilent Chemstation Driver 2.1.3

Warranty

March 2007

CTC Analytics AG reserves the right to make improvements and/or changes to the products and programs described in this User Manual at any time without notice.

CTC Analytics AG makes no warranty of any kind with regards to this product, including but not limited to, the implied warranties or merchantability and suitability for a particular purpose.

The software described in this User Manual is furnished under a license and may be used only in accordance with such license.

© **2007 CTC Analytics AG**. All rights reserved. Neither this publication nor any part of this publication may be copied, photocopied, reproduced, translated or reduced to any electronic medium or machine readable form without the prior written permission of CTC Analytics AG, except as allowed under the copyright laws.

CTC Analytics AG acknowledges all trade names and trademarks used as the property of their respective owners.

Table of Contents

PAL Cycle Composer
User Manual 7

PAL Driver for
Agilent ChemStation Data System
Installation Guide 33

PAL Driver for
ThermoFinnigan Xcalibur Data System
Installation Guide 63

PAL Cycle Composer

Installation Guide
User Manual

Software Revision 1.5.4

Release History

Software Revision CC1.0	Original Release of Cycle Composer Software
Software Revision CC1.3	Cycle Composer Software compatible with ChemStation and Xcalibur Driver
Software Revision CC1.3.2	Cycle Composer Software compatible with Windows NT 4.0 (Administrator /User rights)
Software Revision CC1.4	Cycle Composer Software compatible with PAL Firmware 2.2.0 or higher (serial communication supported by framing protocol)
Software Revision CC1.5	Software Changes for Cycle Composer: PAL Configuration file "*offline_pal.pol*" eliminated. System will use "*latest_pal.pol*" to recognize the PAL Configuration. Sample List: Status differentiates in-between "*Running*" and "*Preparing*". Limitation of maximum 1000 sample line entries eliminated. Practically unlimited number of sample lines are accepted. "*Agitator Off*": Non-numerical value is accepted. Random access to start existing Sample List. Highlight any line in Sample List to start the sequence again at a selected point. PAL Terminal will be locked at the execution of a Cycle Composer method. Unlock with "*Reset PAL*" Improved handshake with Agilent Chemstation Driver. Start/Stop/Abort situations are reliably executed. New SPME cycle added "*SPME Agitated & Heated – Special Penetration*". Complete Cycle with more flexibility for vial and injector penetrations. Configuration dialog added and enhanced

Table of Contents:

1. Introduction to PAL Cycle Composer 11
1.1 What does it do 11
1.2 System requirements 11

2. Installation and Setup 11

3. Connection to PAL 15
3.1 Running On-line 15
3.2 Running Off-Line 15

4. Initial Setup 16
4.1 Port 16
4.2 Reload PAL Configuration 17
4.3 Choose Method Folder 17
4.4 Status Box 17
4.5 Format Sample List 18

5. Sample List Editor 19
5.1 What does it do? 19
5.2 The Sample List Table 19
5.3 Creating a Sample List in the “Trays” Screen 20
5.4 Running a Sample List 21
5.5 Restarting a Sample List 22
5.6 Importing a Sample List from an Excel File
5.7 Other Function Buttons 23

6. Method Editor 24
6.1.Single Step Methods 24
6.2 Multi Step Methods 25
6.3 Composing a new Method 25
6.4 Method Description 27
6.5 Testing with Run and Step 27
6.6 Saving Changes 27

7. Macros for Cycle Composer Software 28
7.1 Standard Macros 28
7.2 Macros for HTS / HTC / LC PAL 29
7.3 Macros for GC PAL 29
7.3 Macros for Combi PAL 30

8. PAL Folder Structure 32

9. File Extensions 32

1. Introduction to PAL Cycle Composer

1.1 What does it do?

Cycle Composer is a 32 Bit Windows based software. Cycle Composer allows customization of sampling cycles for the CTC PAL System. It enables the user to go beyond the capabilities of the local stored LC, GC, Headspace and SPME cycles.

Virtually any conceivable sequence of operations can be generated and saved as Cycle Composer (CC) Methods. The program consists of a Method Editor in which the processing of a sample is defined, and a Sample List Editor in which a sample sequence is created in a tabular format where assignments to the Methods to be run and location of the samples are made.

The program accesses the PAL directly via the serial port, obtaining information from the PAL about which objects are available, and presenting these objects as choices in the Editors. When a Sample List is run, the program takes direct control of the PAL, executing the sequence of steps defined in each Method assigned to the current sample.

1.2 System Requirements

Cycle Composer Software Revision 1.5.4 requires PAL Firmware 2.2.0 or higher.

2. Installation and Setup

Note: Administrator access privileges are required to install PAL Cycle Controller.
It is necessary to exit all programs before installing the CC software.

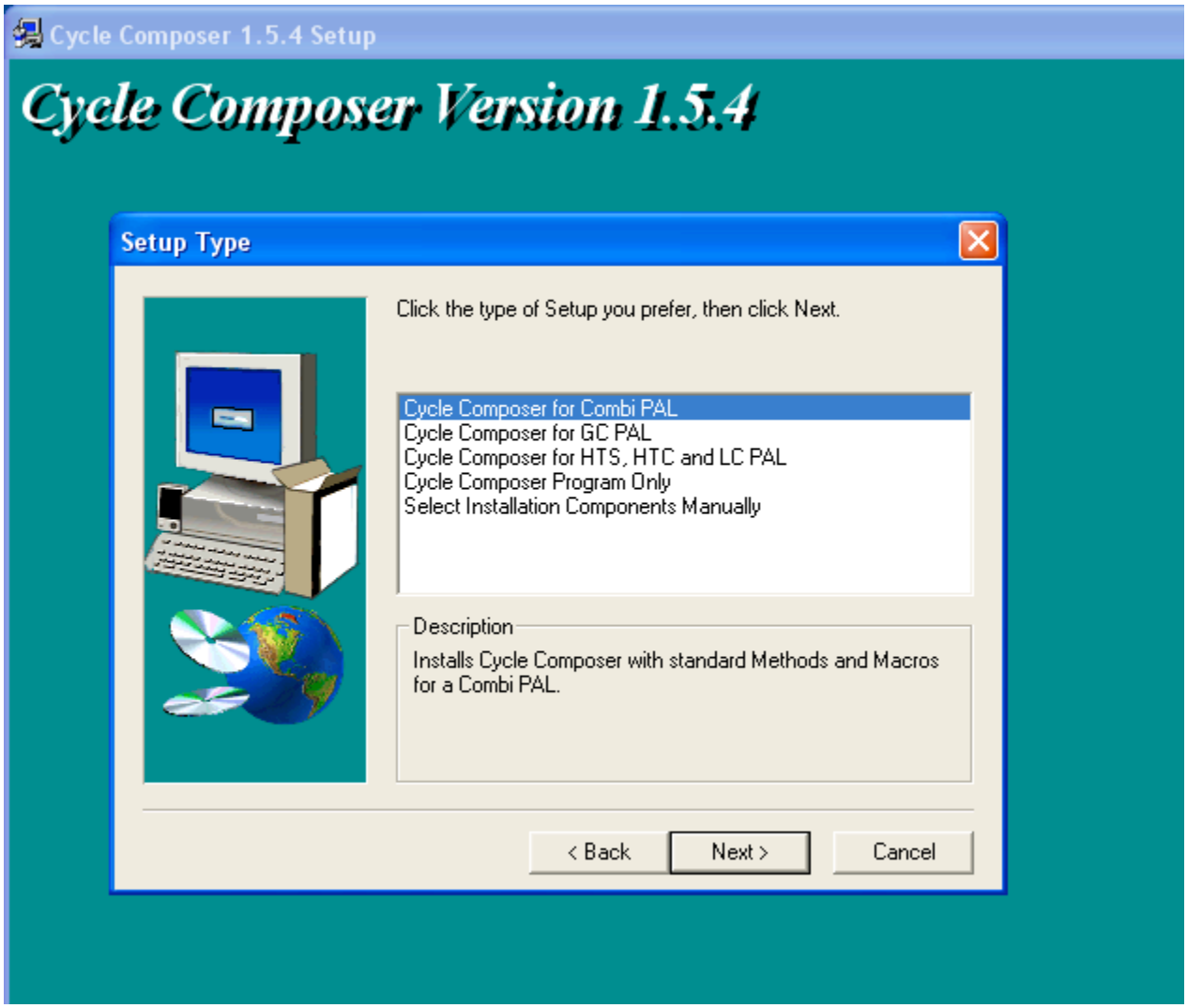
The program is compatible with Windows 98SE, Windows 2000, Windows XP and Windows Vista.

To install the software, place the CD-ROM in the CD drive browse to the folder "*Cycle Composer 1-5-4*". Double-click the file "*CycleComposer1-5-4Inst.exe*" to run the installation program

Note:
CTC Analytics advises to check always the "*Readme.txt*" file on the CD-ROM for any latest information.

After consenting to the Licensing agreement, the user name, the organization name and the serial number have to be entered. The serial number is printed on the backside of the CD-ROM packaging. The software serial number is case dependent. Be sure to use ALL CAPS.
Installing an **Upgrade Version** requires that one of the previous version is installed on the hard disk. During the installation process the software will check for an existing CC version. If the software can not detect a CC version, the installation process will be stopped automatically.

The operator is asked which options shall be installed:



Cycle Composer for GC PAL

Installs Cycle Composer with Standard Methods and Macros for a GC PAL and creates a shortcut of the program in the Start menu.

Cycle Composer for Combi PAL

Installs Cycle Composer with Standard Methods and Macros for a Combi PAL and creates a shortcut of the program in the Start menu.

Cycle Composer for HTS, HTC and LC PAL

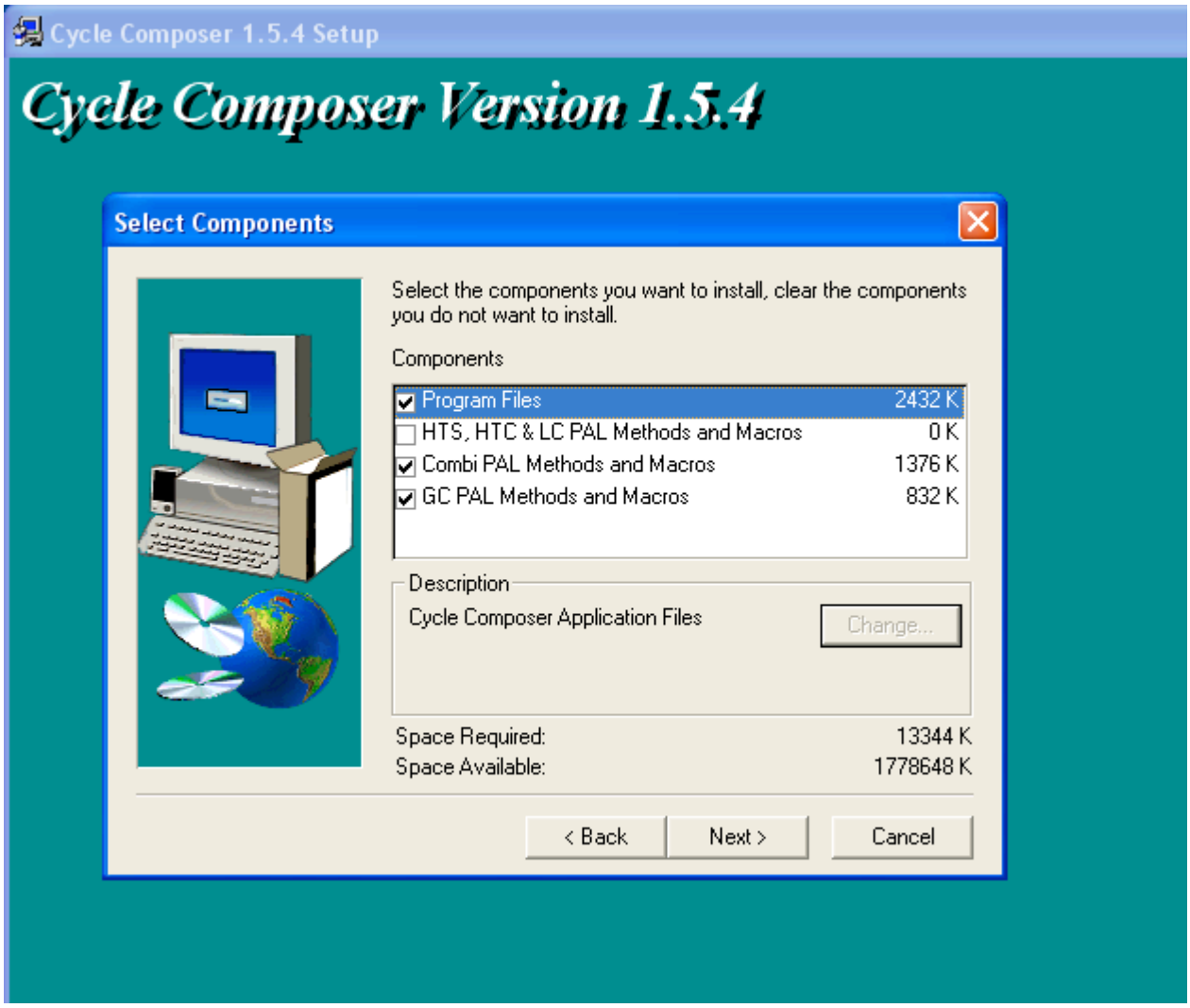
Installs Cycle Composer with Standard Methods and Macros for a HTS, HTC or LC PAL and creates a shortcut of the program in the Start menu.

Cycle Composer Program Only

Cycle Composer Program Files only. After installation use File/Import to load custom Methods and Macros.
This option can be used in an upgrade situation. If the user has made specific changes to existing Standard Macros and saved those with the same name, these would be overwritten by the standard installation process (selecting the options GC PAL or Combi PAL or HTS/HTC/LC PAL). Using this installation option will install the Cycle Composer program files only.

Select Installation Components Manually

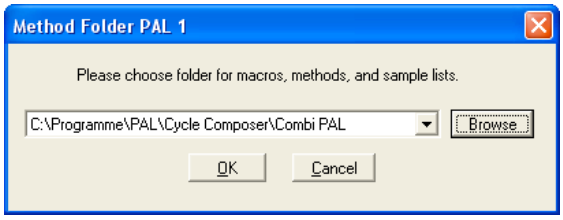
Customized installation.
Can be used if you want to add Methods and Macros for a second type of PAL after initial installation.



After entering the location for the Program Icon folder, the installation will progress automatically.

Setup will place a program icon on your desktop.
Click the "*Finish*" button to complete the installation process.

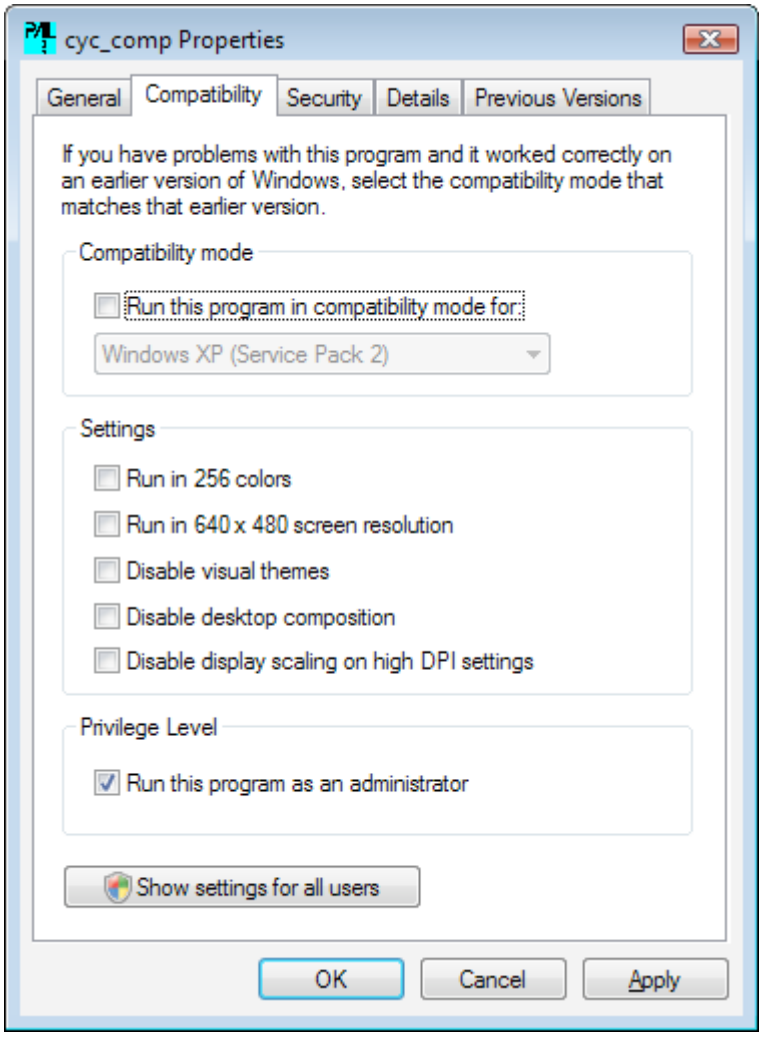
If manual installation has been selected, at the first program start a dialog box will prompt the user to select the path where the Cycle Composer files are stored:



Windows Vista

To use Cycle Composer with Windows Vista, proceed as follows:

- Log in as administrator
- Navigate to the Cycle Composer folder (usually *C:\Program Files\PAL\Cycle Composer*)
- Right click the file "*cyc_comp.exe*"
- From the drop down menu select "*Properties*"
- Select the tab "*Compatibility*"
- Check the option "*Run this program as an administrator*"
- Close the properties window



Cycle Composer is now able to write to the Cycle Composer folder and can also be run as a regular user without administrative rights.

3. Connection to the PAL

3.1 Running On-line

When the CC program is started, it checks the available serial ports for the presence of a PAL.
If one is found, then all the objects on the PAL are uploaded and a message on the Status line displays "*nn objects loaded from PAL*".
If there is a mismatch with the serial port setup or no PAL connected an information message is displayed stating that the program will run off-line.
See chapter 4.1 how to select the correct COM port.

Each time the program successfully connects to a PAL, the set of loaded objects is saved to a disk file called "*latest_pal.pol*".
The program will check for consistency between the set of objects loaded and those required by each Method. Any objects used in a Method which are missing in the PAL are reported in a warning message.

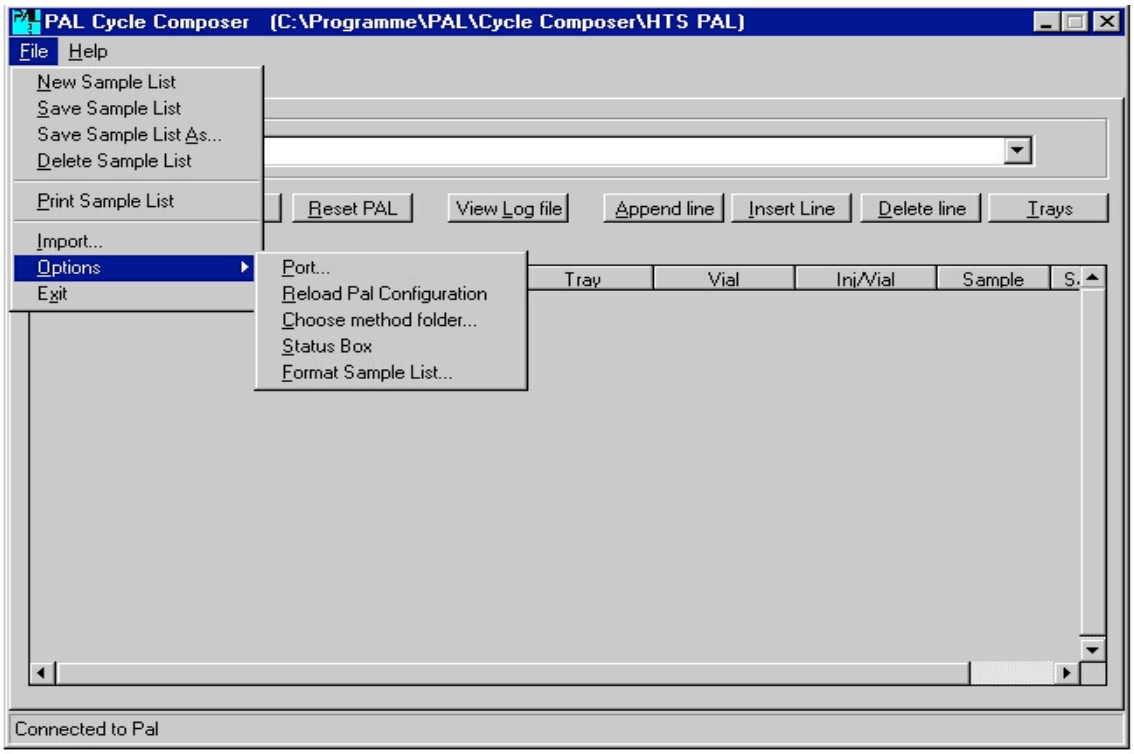
3.2 Running Off-line

If there is no PAL detected when the program starts, it will load a set of objects from the file called "*latest_pal.pol"*.

The file "*offline_pal.pol*" has been eliminated with this Revision 1.5 to simplify the CC handling in an off-line situation.

4. Initial Setup

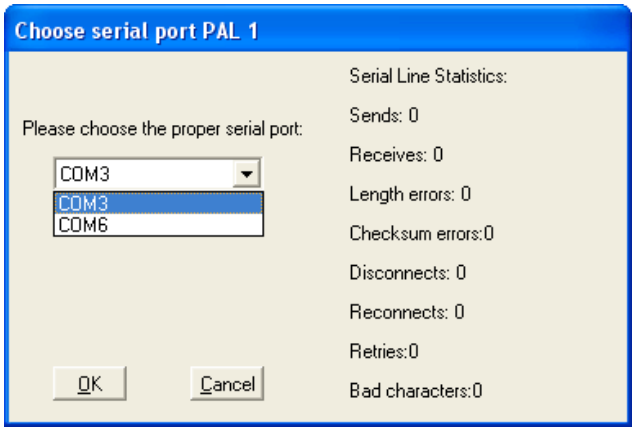
There are 5 setup options available from Main screen under File menu:



4.1 Port

This setup option allows the user to define which COM port on the PC is to be used to connect to the PAL. By default COM1 is used. Connect this port to the serial port SER1 of the PAL using the null modem cable provided.

Switching the port reconnects to the PAL and loads the configuration.



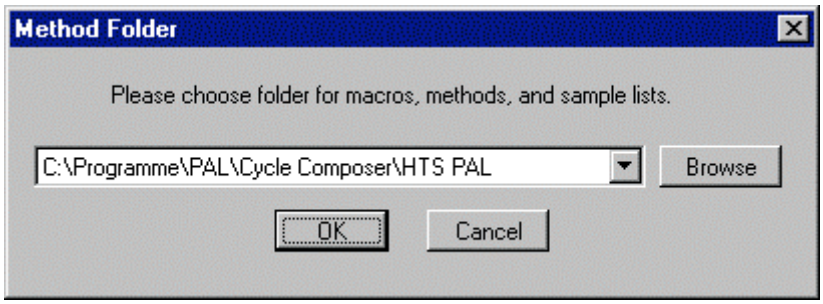
If some other program is using the selected COM port, an error message is shown. Close that program or select a different port.

4.2 Reload PAL Configuration

If any changes are made to the PAL configuration while Cycle Composer is running, these changes are not transferred to the PC and the program is unaware of them. It is necessary either to close and restart Cycle Composer, or select this option from the menu.

4.3 Choose Method Folder

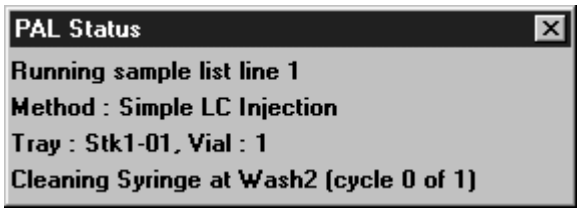
After installation the program will store Macros and Methods to the default path beneath the Cycle Composer folder. Depending on which PAL configuration has been selected this will be the folder "*HTS PAL*" or "*Combi PAL*". It is possible to select a different path to save and load Methods and Macros using menu "*File/Options/Choose method folder…*".



The most recent locations are saved and can be selected in the selection list. Click the "*Browse*" button to search for a different folder not available in the selection list.
Changing to a different folder also reloads the PAL configuration. This is especially useful when working offline with different configurations.

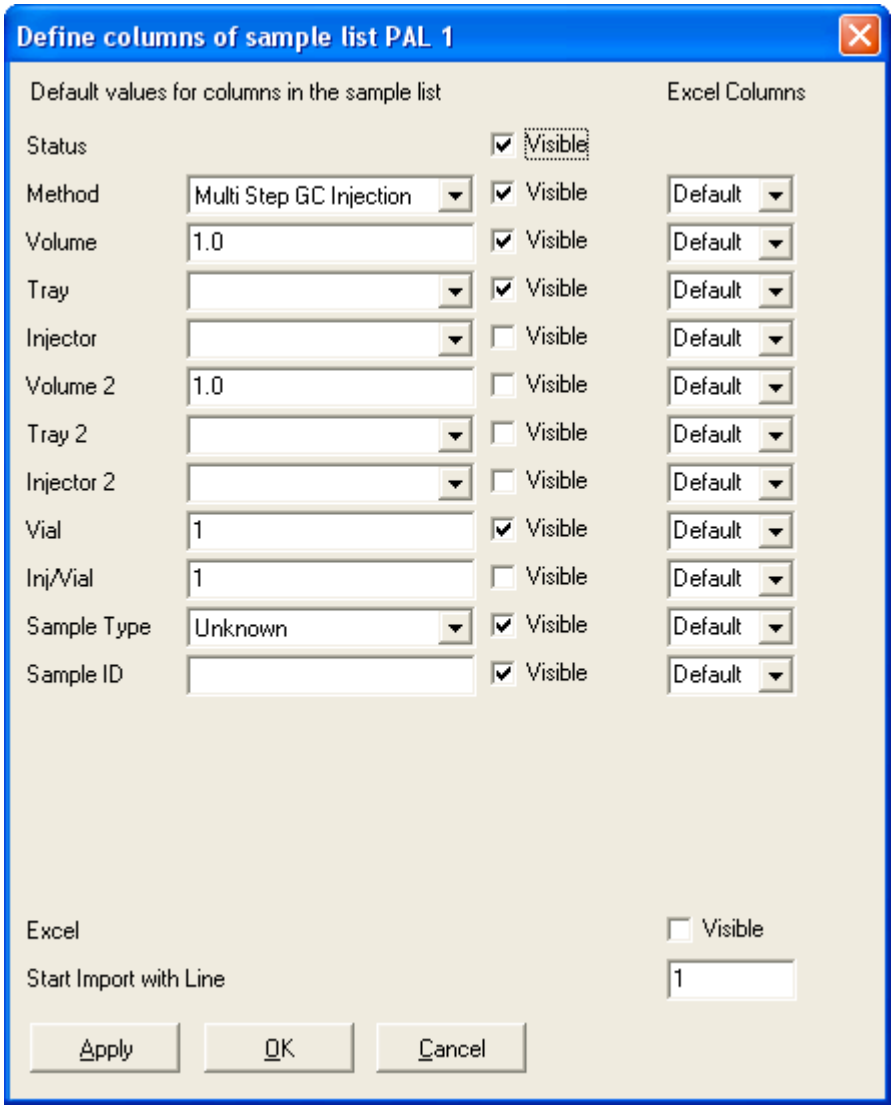
4.4 Status Box

Activating this option displays a status window which informs about the sample number of which tray is processed, the Method being used and which processing step is executed.



4.5 Format Sample List

This option allows the operator to select which Sample List columns are visible for editing in the Sample List table, as well as which defaults are used for all fields. After installation, the fields for Method, Volume, Tray, Vial, Sample Type and Sample ID are marked as visible.



In the "*Excel Columns*" fields the correspondence between Cycle Composer sample list column and the column of an imported Excel file can be selected. If the Excel sheet contains some header lines above the sample list the first sample line can be selected in "*Start Import with Line*".

5. Sample List Editor

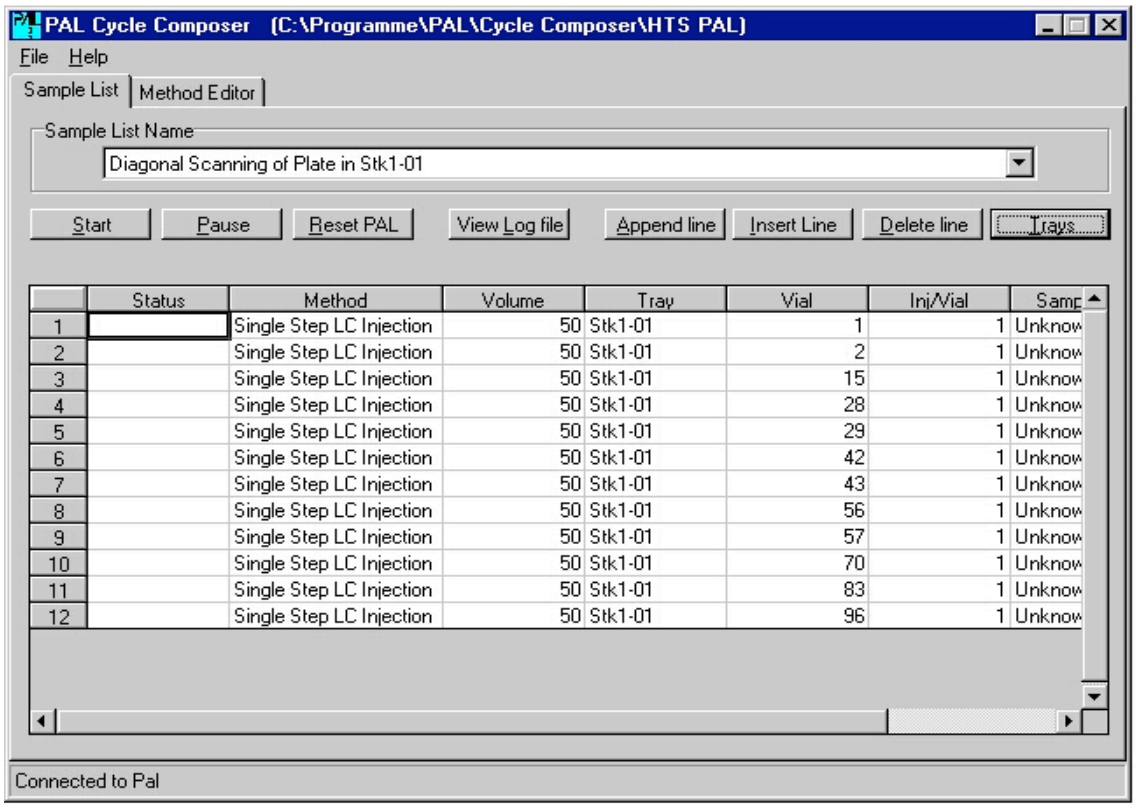
5.1 What does it do?

The sample list editor is the main interface of the CC program. It allows the operator to generate a sequence of samples to be run and initiate the run on the PAL. The Sample List is either created directly line by line or is generated using a graphical representation of the trays.

All file and setup operations are accessed via the "*File*" menu. These include creating a new Sample List, saving with a different name, printing etc. Available saved Sample Lists are accessed from the pull-down list next to the title box "*Sample List Name*".

5.2. The Sample List Table

Each line in the Sample List represents a sample in the sequence and contains fields for the controlling parameters. The table can be edited directly. Values for numeric fields must be typed in. The Method, Tray and Injector fields are filled by selecting the desired item from the pull-down lists. Use the TAB key to go to the next field. All fields must have a valid entry.



Pressing TAB at the last field of the last line creates a new line with the same content as the previous one but with the sample number incremented. Also pressing the down arrow key when a field in the last line is selected appends a new line.

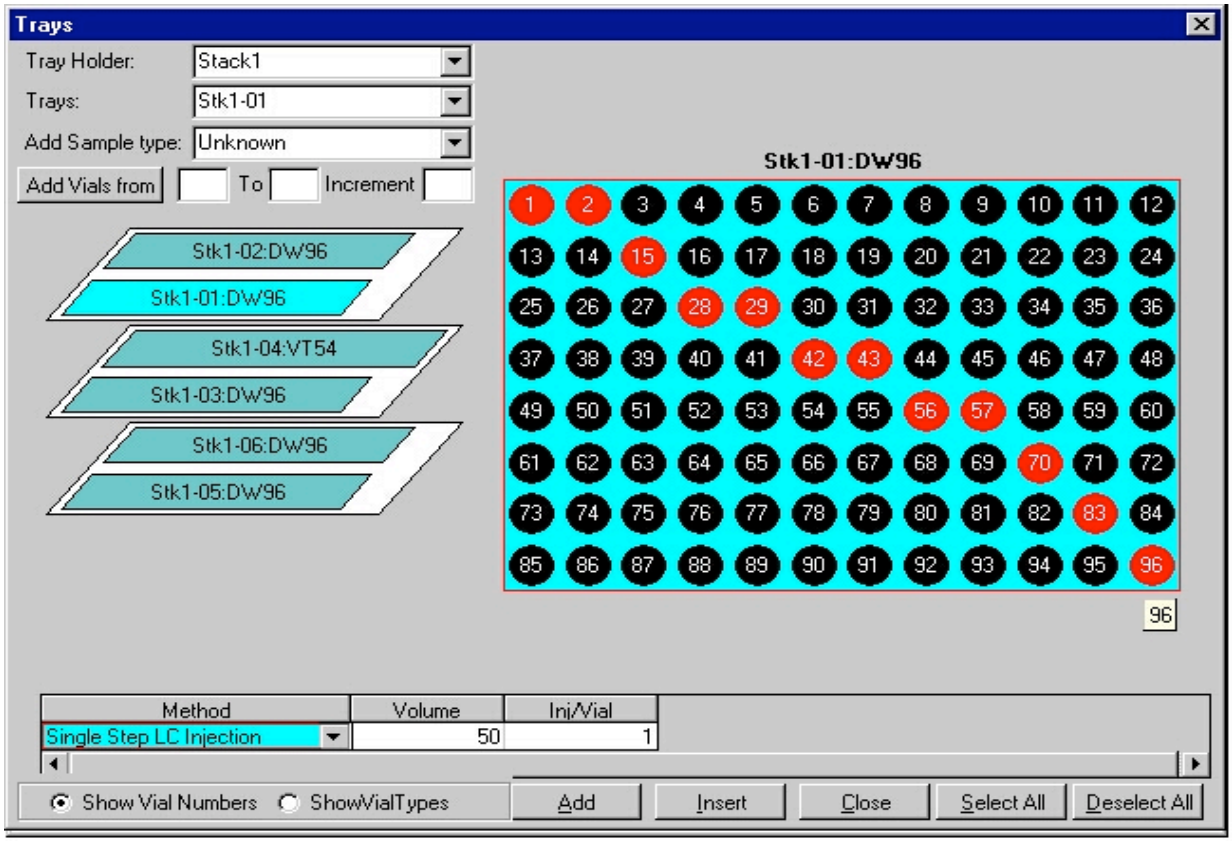
Single or multiple lines can be cut out (CTRL-X) or copied (CTRL-C) and inserted at another position (CTRL-V). Select the lines by clicking on a line number and dragging up or down.

A single field may be copied and applied to the whole column. First copy the field then click on the column header to select the column and press CTRL-V.

5.3 Creating a Sample List in the "Trays" Screen

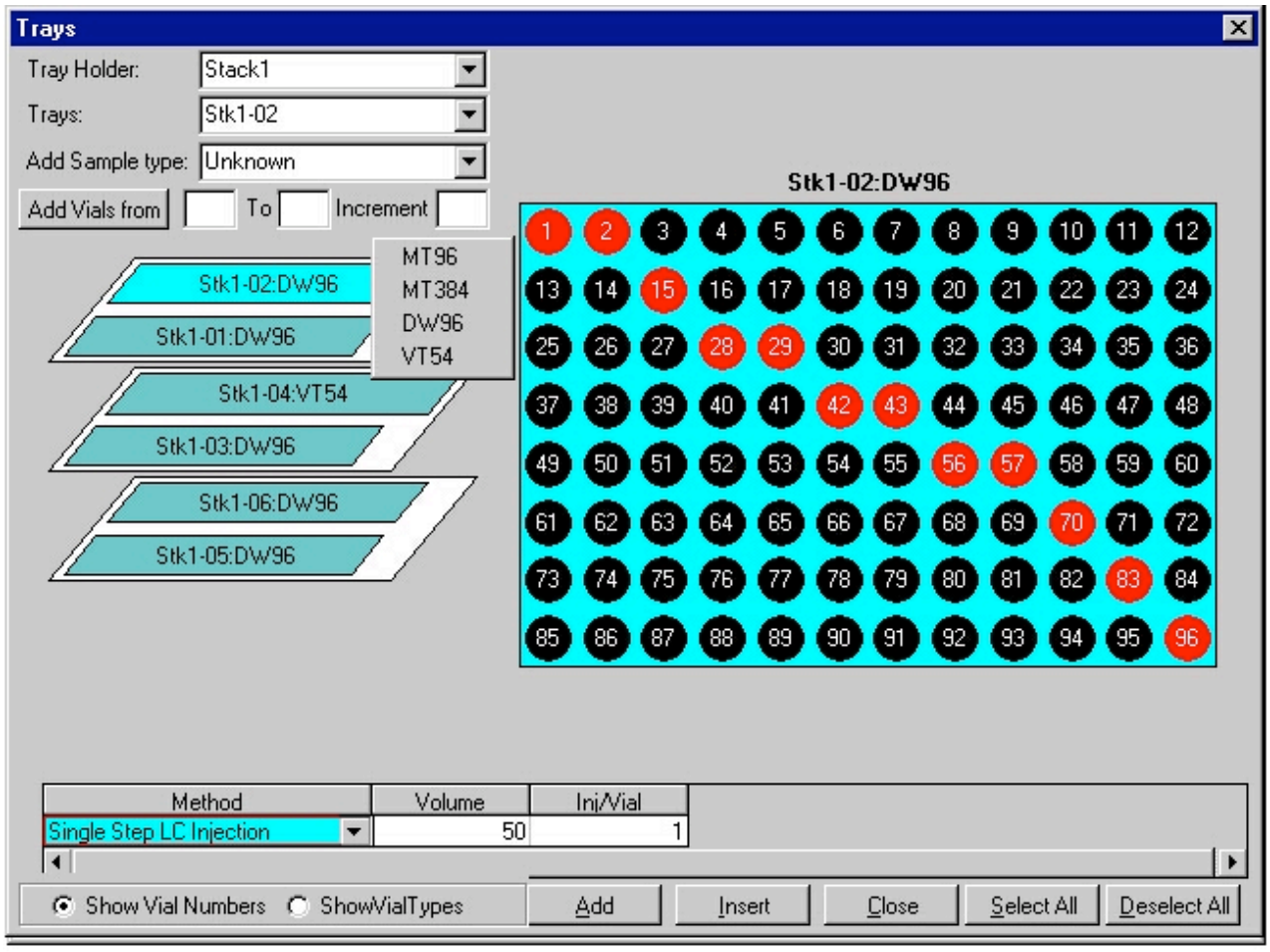
By clicking on the "Trays" button an interactive screen allows the user to easily implement a complex sample list using a graphic interface represented by a map for each of the available trays.

First, select the tray holder from the pull-down list. Then click on the representation of the required tray. A map of this tray then appears showing all the available sample positions.



Select individual or groups of samples on the tray by clicking on their positions or clicking and dragging across multiple positions. Make selections in the other fields for the Method to be run, Injector and the volume etc. Finally click on the "*Add*" button to add the samples to the end of the Sample List or the "*Insert*" button to add lines above the selected line.

If the tray type of the desired tray is not the correct one, right-click on the tray symbol on the left side and select the correct one out of the list of all available tray types which fit to this tray.



5.4 Running a Sample List

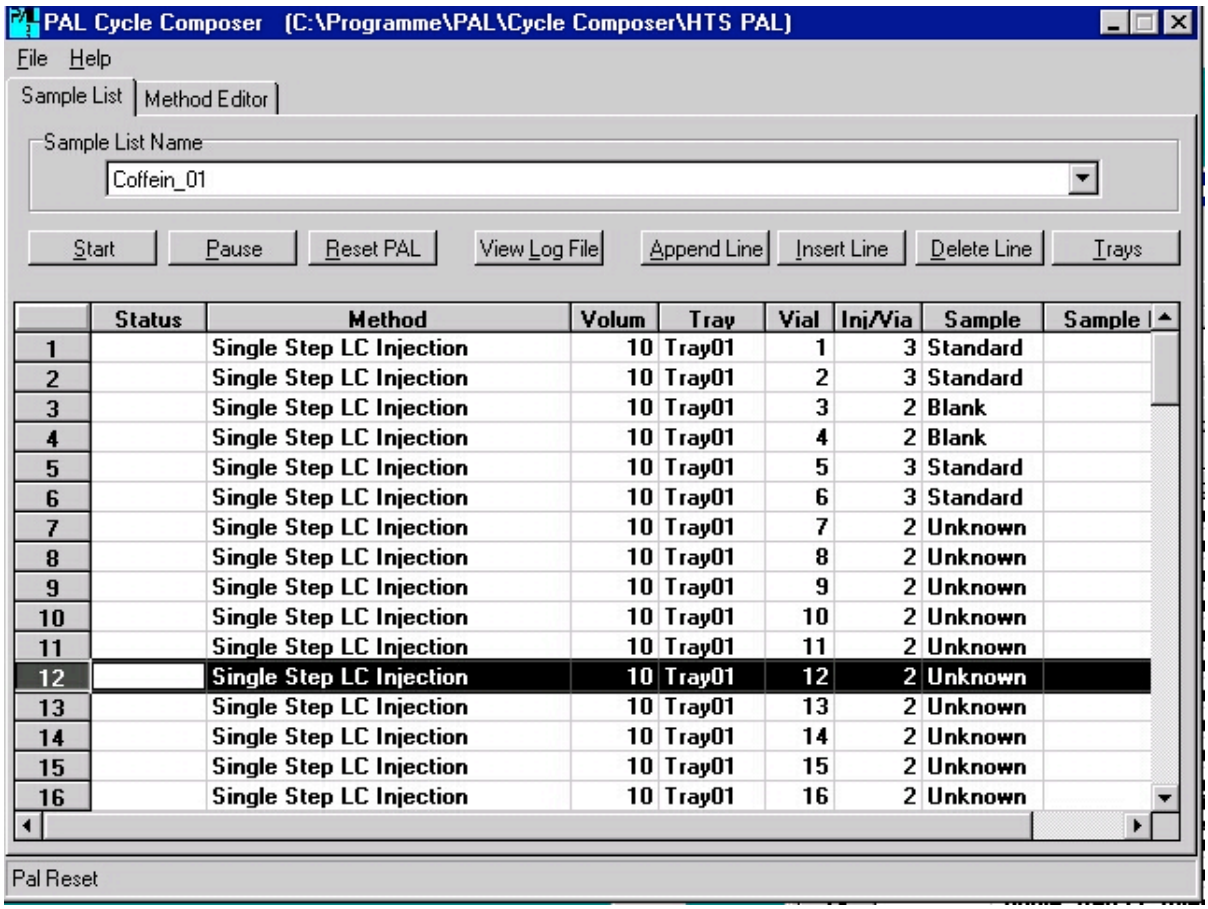
A Sample List is ready to run after one or more lines are entered. To start the run click the "*Start*" button. The PAL will process each line in the list until all are completed. "*Pause*" will temporally halt the PAL without aborting the run.

The Status field will display *"Running"*, after completion of the sample handling or injection step, the Cycle Composer will continue to the next line and would be ready for the next processing step, indicating *"Preparing"* as status.

5.5 Restarting a Sample List

An existing Sample List can be executed again, this will start the list from line 1.

If the user wishes to start the Sample List from a selected line, highlight the line and press "*Start*". All the lines below including the selected line will be processed.
If a single sample (line) only shall be executed, process as described above and in conjunction with the random access line press the "*Pause*" button. This operation allows the user to start at a selected sample line without editing the existing Sample List.



	Status	Method	Volum	Tray	Vial	Inj/Via	Sample	Sample
1		Single Step LC Injection	10	Tray01	1	3	Standard	
2		Single Step LC Injection	10	Tray01	2	3	Standard	
3		Single Step LC Injection	10	Tray01	3	2	Blank	
4		Single Step LC Injection	10	Tray01	4	2	Blank	
5		Single Step LC Injection	10	Tray01	5	3	Standard	
6		Single Step LC Injection	10	Tray01	6	3	Standard	
7		Single Step LC Injection	10	Tray01	7	2	Unknown	
8		Single Step LC Injection	10	Tray01	8	2	Unknown	
9		Single Step LC Injection	10	Tray01	9	2	Unknown	
10		Single Step LC Injection	10	Tray01	10	2	Unknown	
11		Single Step LC Injection	10	Tray01	11	2	Unknown	
12		Single Step LC Injection	10	Tray01	12	2	Unknown	
13		Single Step LC Injection	10	Tray01	13	2	Unknown	
14		Single Step LC Injection	10	Tray01	14	2	Unknown	
15		Single Step LC Injection	10	Tray01	15	2	Unknown	
16		Single Step LC Injection	10	Tray01	16	2	Unknown	

5.6 Importing a Sample List from an Excel File

Using menu "*File/Import Excel Sheet*" it is possible to import a sample sequence from an Excel sheet into the Cycle Composer sample list. The correspondence between Excel column and sample list column has to be set correctly in "*Format Sample List*" window (see chapter 4.5).

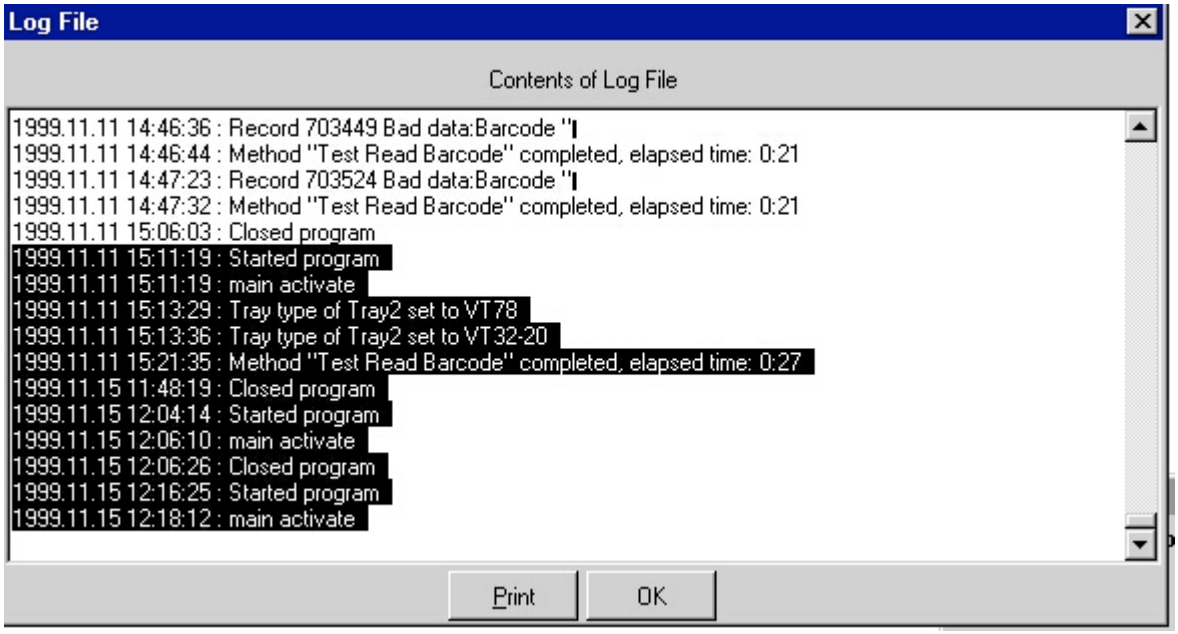
5.7 Other Function Buttons

"Reset PAL" is available if a list is not in progress. It allows the user to easily re-initialize all the devices on the PAL. This is useful if a run has been aborted and the injection head or syringe are not in the home position.

Another function of the *"Reset PAL"* is to unlock the local terminal. For Utilities Functions, like change syringe, activate valve and others, it is necessary to utilize the local terminal. Starting the Cycle Composer method again, the local terminal will be locked automatically.

"*Insert Row*" and "*Delete Row*" button allows quick rearrangement of the Sample List Table. *"View Logfile*" opens a text file which contains an activity log for all Cycle Composer sessions. This file may be printed out for documentation purposes.

The content of the file is the full history. To print out a specific section only, one can highlight the lines of interest and print those selectively.

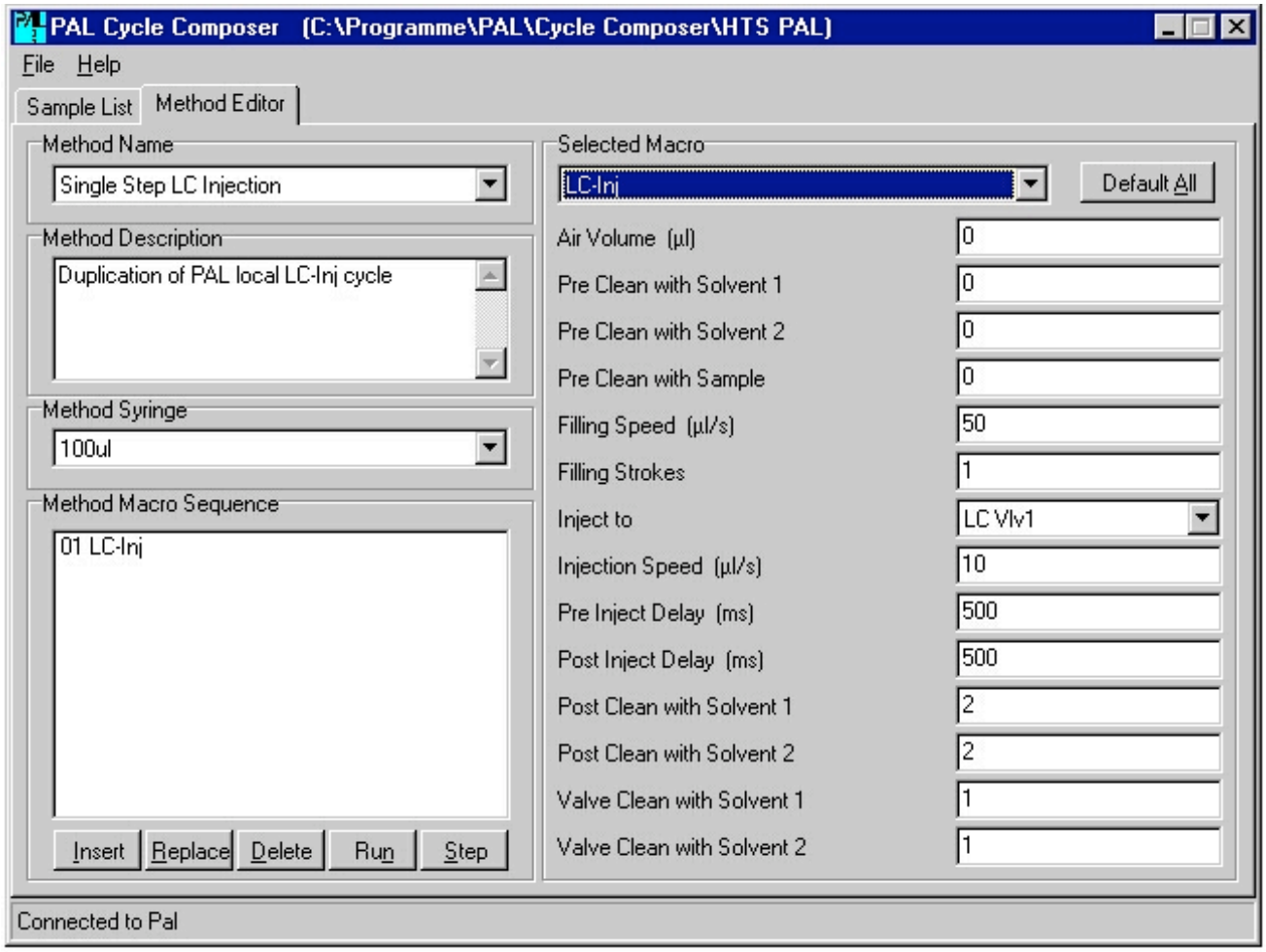


6. Method Editor

6.1 Single Step Methods

Single Step Methods use a single Macro which has the complete cycle built into it. All values which control the cycle are shown on a single page.

A typical Single Step Method is provided with the Cycle Composer program. It mimics the on-board PAL Method for the selected instrument type. A number of sampling parameters can be changed to optimize the Method to suit the conditions of the run. When modified in this way it can be stored with a unique name.



Because a Single Step Method consists of a single Macro with associated parameter values the sequence of processing steps can not be changed at this level. But often it is possible to change some aspects of the cycle by setting some parameters accordingly. In the example above cleaning before injection is skipped by setting the three "*Pre Clean*" parameters to zero.
In the description of standard Macros later in this guide all Macros which can be used for a Single Step Method are marked with "*Complete Cycle*".

6.2 Multi Step Methods

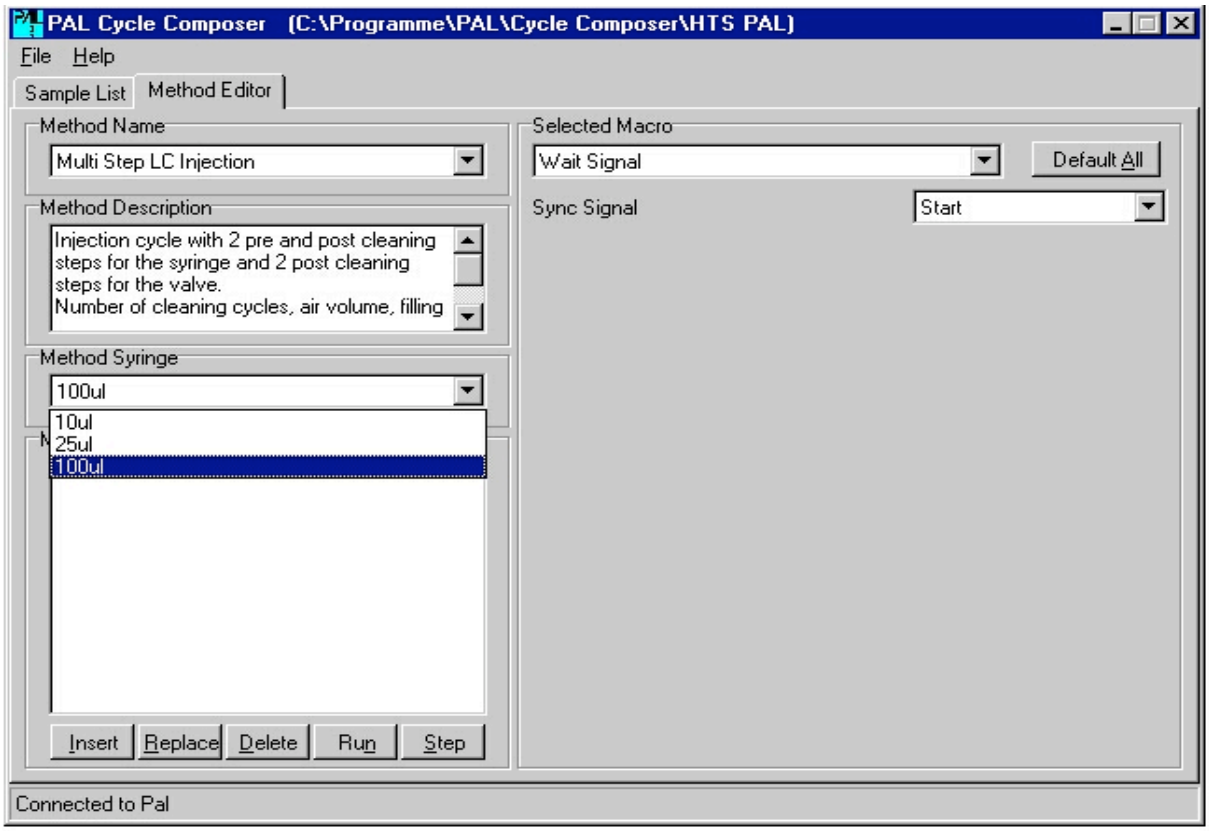
A Single Step Method has a fixed sequence of PAL operations which can not be altered by the user. If this is not appropriate for the application the user can compose his own sequence. Small building blocks, so-called Macros, are combined to construct a new sampling cycle. A Multi Step Method consists of a sequence of Macros each having its own set of parameter values.

A set of standard Macros is installed together with the Cycle Composer program. A list and description of these is provided in chapter "*Standard Macros*".

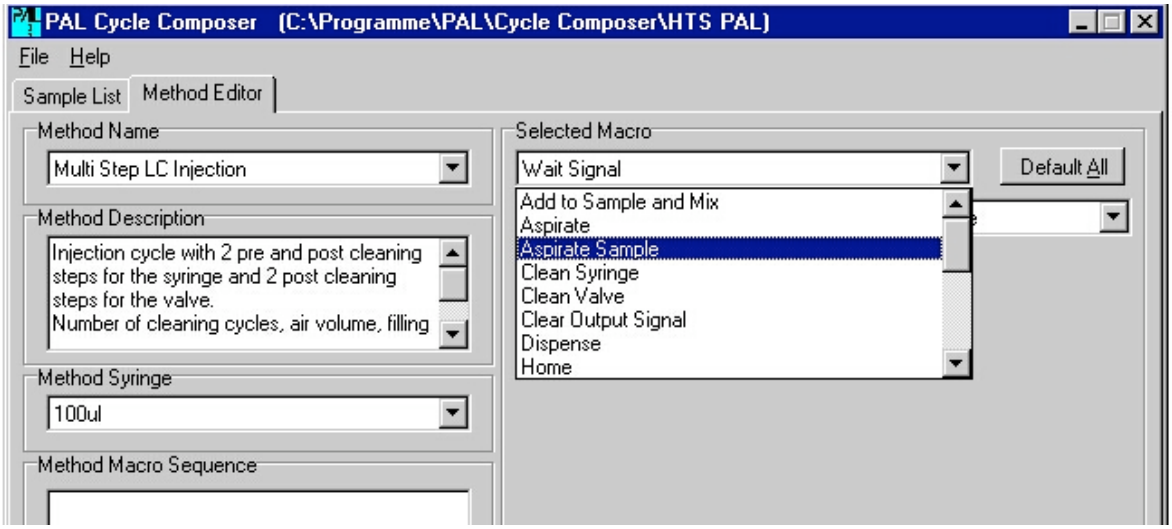
6.3 Composing a new Method

To create a new Multi Step Method, select "*New Method*" under the "*File*" menu, and give it a name.

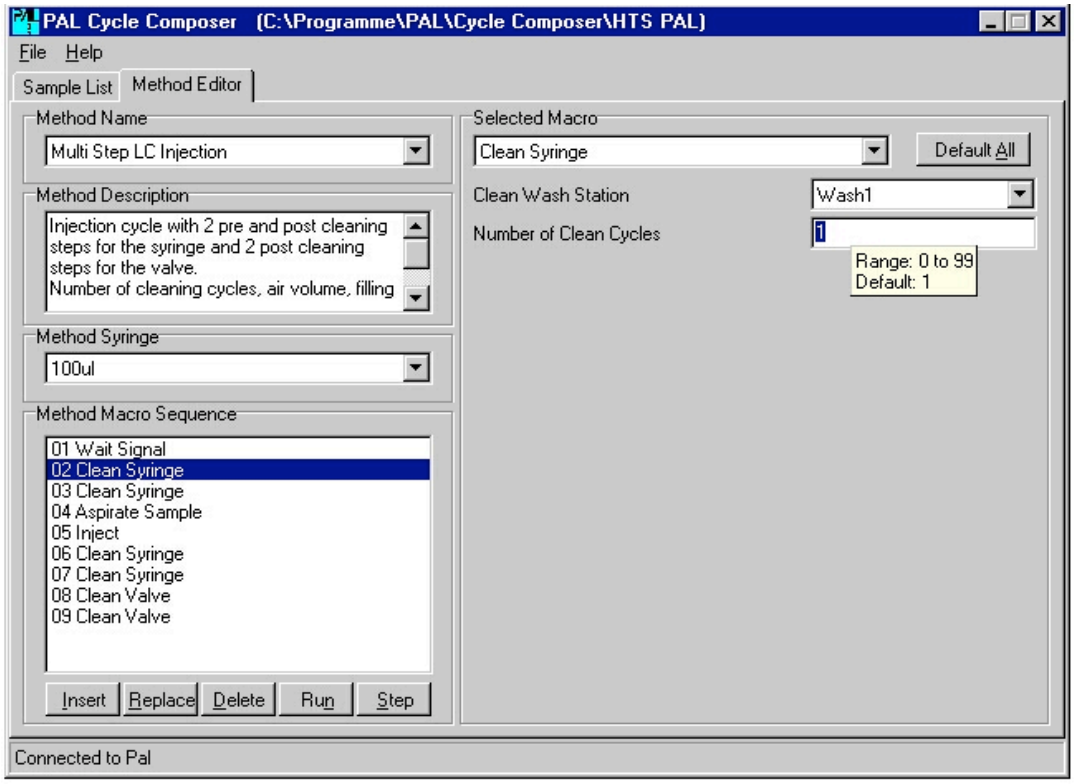
Then select a syringe to be used for this Method. It is essential that the syringe is selected before Macros are added to the Method. The selected syringe sets different default values and ranges for volumes and flow rates. It is possible to change the syringe for an existing Method but it may happen that Macro values are no more within the valid range and have to be adjusted.



Now start to compose the sequence of operations in the box labeled "*Method Macro Sequence*" using the available Macros from the list on the right side labeled "*Selected Macro*". Moving the cursor to the Macro name displays a hint with a short description of the Macros function.



After a Macro has been selected modify any required parameters presented in the table beneath it on the screen. When these are complete, select the "*Insert*" button under the sequence table and the Macro will be placed in the sequence below the current position. Repeat this process for each step in the sequence.
If a parameter for any Macro has to be modified, select the Macro in the sequence for which the modification is to be made, then change the desired value. If the Macro itself
is not changed then the new value is automatically applied. Moving the cursor to the parameter field displays a hint with the minimum, maximum and default value.



Clicking the right mouse button when the cursor is on a numeric field displays a list of possible special values: The default value and special Syringe and Sample List related values. Which values are shown depends on the unit of the actual field. Values starting with "*SYR*" reference the methods syringe (min and max volumes and default plunger speeds) and values starting with "*SL*" reference the Sample List columns (Volume, Tray, Vial, Injector, etc).

If a different Macro needs to be put in an existing sequence, place the cursor at the location in the sequence where the replacement is to be made, then select the new Macro, set the parameters as desired and click the "*Replace*" button.

6.4 Method Description

It is important to stress the benefit of a good description for each Method. The description entered in the "*Method Description*" box will provide information to the user in the Sample List screen. These are displayed whenever the user rests the cursor over each Method in the Sample List. Likewise, each Macro contains a description, which will be displayed when the user rests the cursor on the selected Macro in the Method Editor screen.

6.5 Testing with RUN and STEP

When a Method has been created, it can be tested before implementing it into a Sample List by selecting the "*Run*" or "*Step*" button.

The operator is prompted to enter values which are normally passed by the Sample List. These are used to run this test. If Step mode is selected, each Atom sent to the PAL is displayed before it is executed. A Macro may be built of several PAL Atoms. The Macros "*SL Entry*", "*Method Entry*", "*Method Exit*" and "*SL Exit*" are macros which are automatically appended in front and at the end of the method macro sequence. They are used for initialization before the sequence and method and cleanup after the method and sequence.

6.6 Saving Changes

Whenever a Method has been changed, this change is not saved immediately to the disk. This is done explicitly with the menu "*File/Save*" or "*File/Save as...*". If the user switches to the Sample List but did not yet save the Method a dialog box asks if the changed Method should be saved.

7. Macros for Cycle Composer Software

7.1 Standard Macros

Add to Sample and Mix
Aspirate liquid from Liquid Reservoir. Dispense into sample vial specified in Sample List. Mix by selected number of full plunger strokes.

Aspirate
Fill syringe from a vial with Tray Name, Sample Volume, Air Volume, Fill Speed and Fill Strokes specified as parameters.

Aspirate Sample
Fill syringe from a vial with Tray Name, Vial Number and Sample Volume specified in the Sample List and Air Volume, Fill Speed and Fill Strokes specified as parameters.

Clean Syringe
Clean syringe using selected wash station and number of clean cycles. Default values for all other parameters are taken from the syringe or wash

Clear Output Signal
Deactivate the selected Output Signal. The output pin on the interface connector and the active state of the signal are defined in the selected Output Signal object.

Dispense
Dispense syringe content to a selected position using speed Parameters.

Home
The PAL moves the injection head back to home position.

Inject
Inject syringe content to a selected injector with speed, pre and post inject delays and output signal as parameters. Sync signal Inject is waited before injection and timer 1 is started at injection time. If the injector has a valve referenced, it is switched before injection and switched back after injection.

Pulse Output Signal
Activate the selected Output Signal for specified Pulse Time. The output pin on the interface connector and the active state of the signal are defined in the selected Output Signal object.

Set Output Signal
Activate the selected Output Signal.. The output pin on the interface connector and the active state of the signal are defined in the selected Output Signal object. Use the Macro "*Clear Output Signal*" to deactivate the signal.

Transfer Liquid and Mix
Transfer liquid from source to target. Mix with full plunger strokes.

Transport Vial
Transport vial magnetically from Source Tray to Target Tray.

Wait Signal
Wait for Sync Signal. The input pin on the interface connector and the active state of the signal are defined in the selected Sync Signal object.

Wait
Wait for selected time delay.

7.2 Macros for HTS / HTC / LC PAL

Clean Valve
Rinse valve with solvent from selected wash station. Default values for all other parameters are taken from the syringe or wash station object.

Switch Valve to Inject
Switch selected valve to inject position after selected time since last injection.

Switch Valve to Load
Switch selected valve to load position after selected time since last injection.

LC -Inj
Complete Cycle
Duplication of PAL's local LC injection cycle. Tray Name, Sample Number and Sample Volume are taken from the sample list.
This Macro contains the complete sampling cycle - all parameters are on a single page.

7.3 Macros for GC PAL

GC-Inj
Complete Cycle
Duplication of PAL's local GC liquid injection cycle. Tray Name, Sample Number and Sample Volume are taken from the sample list.
This Macro contains the complete sampling cycle - all parameters are on a single page.

7.4 Macros for Combi PAL

Start Agitator
Starts the Agitator with selectable speed, run and pause times.

Wait Agitator
Stops the Agitator after a selectable run time.

Set Temperature
Sets the temperature of a heated object to a selectable value. The macro returns before the temperature is reached.

Wait Temperature
Wait until a specified temperature of a heated object is reached.

GC-Inj
Complete Cycle
Duplication of PAL's local GC liquid injection cycle. Tray Name, Sample Number and Sample Volume are taken from the sample list.
This Macro contains the complete sampling cycle - all parameters are on a single page.

Headspace
Complete Cycle
Set temperatures of Agitator and syringe to the desired values. After temperatures have stabilized the vial is transported into the Agitator, activates the Agitator and waits for a selectable incubation time. Then the sample is taken out of the headspace and injected. The vial is moved back into the sample tray and the syringe is flushed.
To be able to overlap the incubation time with the GC Runtime the GC Ready signal is not checked before the vial is inserted into the agitator, but it is checked before injection. The Macro is terminated after a delay time of (GC Runtime - Incubation Time) which started at the injection moment. For a GC Runtime which is shorter than Incubation Time the next vial is inserted immediately. If the GC Runtime is longer than Incubation Time the vial is inserted with such a delay that it will be incubated for the correct time when the GC gets ready.
This Macro contains the complete sampling cycle - all parameters are on a single page.

SPME Agitated & Heated
Complete Cycle
Set temperature of Agitator to the desired value. After temperature has stabilized the vial is transported into the Agitator. If "*Pre Incubation*" time is selected, the sample is shaken and heated. The movement of the Agitator is stopped, the needle guide is blocked (Exp Fiber) and the SPME–Fiber is inserted into the vial. The vial penetration for the fiber is fixed, not selectable by the user. The Fiber is exposed into headspace or the liquid phase.
The Agitator is started and moves on a fixed speed, slowest possible speed to yield in a round movement. The sample is heated and the equilibrium will be reached during the selected time "*Extraction Time*".
The SPME-Fiber is retracted, the synchronization signal is awaited and the needle guide will be released. The Fiber is moved to the selected GC Injector, and the analytes will be thermally desorbed. The Fiber remains in this position until the timer of "*Desorption Time*" reaches Zero. The Fiber is retracted and the vial is taken back into position.
The Macro contains the complete sampling cycle – all parameters are on a single page.

SPME Agitated & Heated - Special Penetration

Complete Cycle

This macro is a duplication of the macro "*SPME Agitated & Heated*" with the differences that the user has more flexibility with the parameters "*Vial Needle Penetration*", "*Vial Fiber Exposure*", "Injection Needle Penetration" and "*Injection Needle Exposure*".
The Macro contains the complete sampling cycle – all parameters are on a single page.

SPME Heated

Complete Cycle

This Macro has the exact same structure as the Macro "*SPME Agitated & Heated*". The only difference is that the analytical sample is heated only and not agitated. The Agitator is turned off during the "*Pre Incubation Time*" as well as during the "*Extraction Time*".
The Macro contains the complete sampling cycle – all parameters are on a single page.

SPME Out of Tray

Complete Cycle

The SPME-Fiber is moved to the selected vial in the corresponding Tray, is inserted and exposed for the desired "*Extraction Time*" to reach the equilibrium. The Fiber is retracted and the synchronization signal is awaited. The Fiber is moved to the selected GC Injector. The analytes are thermally desorbed and the Fiber remains in this position until the timer for the "*Desorption Time*" reaches Zero. The Fiber is retracted and the head moves back to home position.
This Macro does not use the Agitator at all. The sample preparation is done at ambient temperature (or at selected temperature with a cooled/heated sample Tray).
The Macro contains the complete sampling cycle – all parameters are on a single page.

Bakeout Fiber

Complete Cycle

This Macro is used in combination with the SPME Fiber Bake-out Station. After the thermal desorption of the analytes, the SPME-Fiber is moved to the Bake-out Station. The Fiber is exposed and conditioned during the selected "*Bakeout Time*". After this time the Fiber is retracted.
[The temperature is set by using the local terminal under Menu/Utilities/Injectors. Select "*NdlHeatr*" and set the desired temperature at "*Standby Temp*".
A constant gas flow protects the Fiber.

8. PAL Folder Structure

The following folder structure is created as default by the install program and is recommended for installing PAL related software on your PC:

C:\ Program Files
\PAL
\Cycle Composer
\GC PAL
\Combi PAL
\HTS PAL

\Loader
\Backup
\Update

Following this format will make trouble-shooting easier and allows to automate some of the update procedures.

9. File Extensions

Following file extensions are used by the Cycle Composer software:

Methods:	*.pme	PAL Method
Macros	*.pma	PAL Macro
Sample List	*.psl	PAL Sample List
PAL Configuration	*.pol	PAL Object List
	latest_pal.pol	Latest Pal Configuration (uploaded Objects from PAL)

PAL Driver for Agilent ChemStation Data System

Installation Guide

Software Revision 2.1.3

Printing History

Edition 1	November 1999	Software Revision 1.0.1
Edition 2	May 2001	Software Revision 2.0.3
Edition 3	June 2001	Software Revision 2.0.4
Edition 4	July 2001	Software Revision 2.0.4
Edition 5	February 2007	Software Revision 2.1.3

Release History

Software Revision 1.0.1

Original Driver for ChemStation Software.

Software Revision 2.0.3

Various improvements and adaptations for new ChemStation Versions:

- Installation Routine checks automatically for 16/32 Bit ChemStation Versions.
- Improved handshake to pause/stop a PAL Cycle Composer sample list in combination with ChemStation.
- Injection Volume and Vial # readable by ChemStation Sequence. Print out via “Miscellaneous Info” or “Sample Info” fields.
- Filenaming improved and equal for all 3 ChemStation versions.
- New created ChemStation method available in drop down menu selection of sample list field “CE Method”.
- LC/MS ChemStation: If an Autosampler of the Agilent Series1100 is configured, it has not to be removed from the configuration to install the PAL System.
- GC6890 and GC-MSD: The Autoprep-Run is activated through the Driver software at the start. Therefore it is not necessary to configure the GC in this mode. The Gas-saver option is fully available.

Software Revision 2.0.4

Variable for ChemStation Report function “InjVol$” added to PALSEQ.MAC.
GC-MSD Version, Parameter ExtraWaitForStart added.

Software Revision 2.1.3

Support for newer Chemstation version has been added

PAL Driver for Agilent ChemStation Data System

Table of Contents:

1. Requirements **37**

1.1 Software Requirements 37
1.2 Workstation Requirements 37
1.3 Synchronization Requirements for the PAL System and the Agilent Instrument 38

2. Installation Procedure **38**

2.1 Order of Installation 38
2.2 Installation for GC / HPLC / LC-MSD 39
2.3 Installation for a GC-MSD 40
2.4 Files used for Agilent ChemStation and Cycle Composer 47
2.5 Injector Naming/Nomenclature 47
2.6 Uninstalling the PAL Cycle Composer Driver for the ChemStation 48

3.Starting PAL Cycle Composer Software in Synchronization with HP ChemStation **48**

3.1 Principle of Synchronization 48
3.2 Starting the PAL Cycle Composer Software 49
3.3 Creating a Sequence 49
3.4 Customize a ChemStation Report Template 52
3.5 Running a Standard (Non-FIA) Sequence (Sample List) 54
3.6 Running a FIA Sequence (Sample List) 56
3.7 Configuring the Chemstation Interface 58

4. Limitations **61**

PAL Driver for Agilent ChemStation Data System

1. Requirements

1.1 Software Requirements

Agilent Number	Version(s)	Instruments	Chemstation Type	Tested
G2070AA	A.06.03 and higher	GC 5890 / 6890	Leochem	Yes
G2170AA	A.06.03 and higher	1100 etc	Leochem	Yes
G2710AA	A.08.04	LC-MS	Leochem	Yes
G2070AA	B.02.01 and higher	GC 5890 / 6890	Leochem	Yes
G2170AA	B.02.01 and higher	1100 etc	Leochem	Yes
G2710AA	B.02.01 and higher	LC-MS	Leochem	Yes
G1701BA	B.01.00	GC-MSD	Mustang	No
G1701BA	B.02.00	GC-MSD	Mustang	No
G1701CA	B.01.00	GC-MSD	Mustang	Yes
G1701CA	C.01.00	GC-MSD	Mustang	Yes
G1701CA	D.00.01	GC-MSD	Mustang	Yes
G1701CA	D.01.02	GC-MSD	Mustang	Yes
G1070CA	D.03.00	GC-MSD	Mustang	Yes
			Cerity	No

- Cycle Composer Software 1.5.4 or higher
- PAL Firmware 2.2.7 or higher

- Optional:
  G2731AA ABI/MDS-Sciex Analyst
  Software for LC/MSD data analysis Revison 1.1.1 or higher

The PAL Driver is running under Windows 2000/XP

ChemStation Cerity is not supported.

1.2 Workstation Requirements

The hardware requirements are given by the HP ChemStation Data System.
Consult the Agilent Manual or a representative of Agilent Technologies

1.3 Synchronization Requirements for the PAL System and the Agilent Instrument

The start/stop/ready signals between the PAL System and the Agilent Instrument (GC, HPLC or GC/MS) is synchronized via hardware signal connection.
Use the PAL connector “Interface 1” and the corresponding Agilent Remote connector.
An appropriate interface cable is available from CTC, P/N: Cbl HP6890

The setup for the PAL Synchronization Signals requires the following steps:

1.) Change the remote start signal from “*Immediat*” to “TTL-In1”
Path: Menu / Setup / Objects / Sync Signals / Start
Action: Change the “Source” from “*Immediat*” to “TTL-In1”.

2.) Change the state of the TTL-1 signal (Agilent specific)
Path: Menu / Setup / Objects / Events / TTL-In1
Action: Change value of “*Active state*” from “*Low*” to “*High*”.

3.) Verify the state of the “Injected” signal (default settings)
Path: Menu / Setup / Objects / Out Signals
Action: Change the value “*Destination from*” from “*Off*” to “*SW-Out1*”

Note: Verify that the AutoPrepRun of the GC 6890 is not active.
Keyboard GC 6890, Path: Configuration / Instrument / AutoPrepRun: “*Off*”.
In this configuration the Gas saver mode is fully active.

2. Installation Procedure

2.1 Order of Installation

1. Agilent ChemStation Software
2. Cycle Composer Software
3. Driver for Agilent ChemStation

Note: It is necessary to exit all programs before installing the PAL Driver software.

To setup the communication between the Agilent ChemStation and the Cycle Composer, it is necessary that the Agilent ChemStation and the Cycle Composer are installed on the workstation. It is advisable to test each software individually. If both programs are working satisfactory the PAL Driver for Agilent ChemStation can be installed.

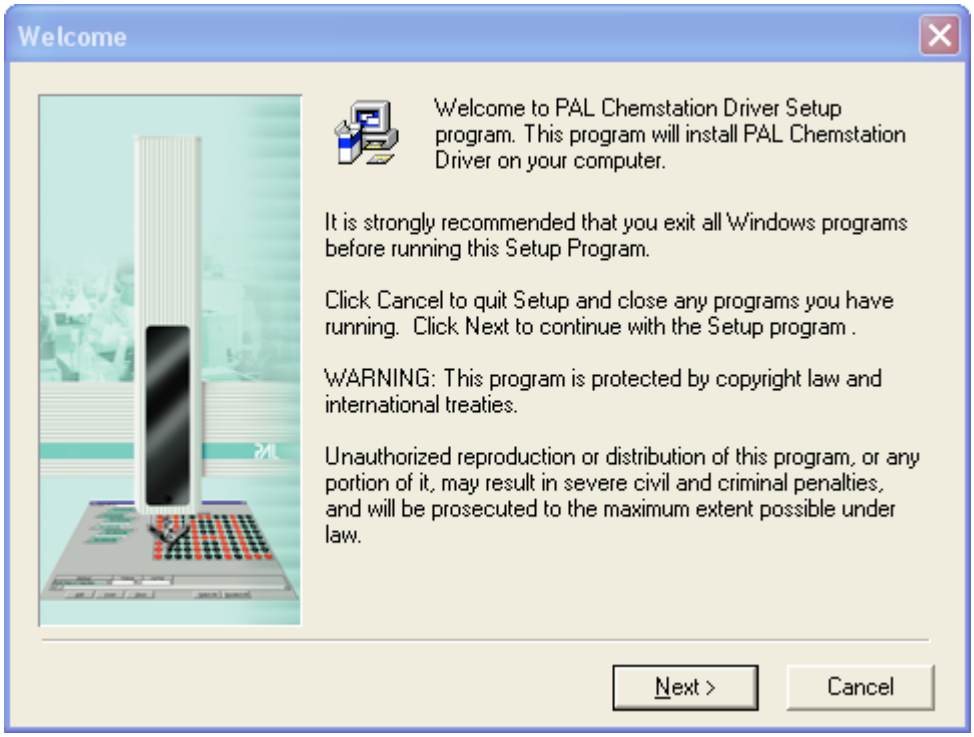
The types of ChemStation environments are:

ChemStation for GC / HPLC
ChemStation for LC-MSD
ChemStation for GC -MSD

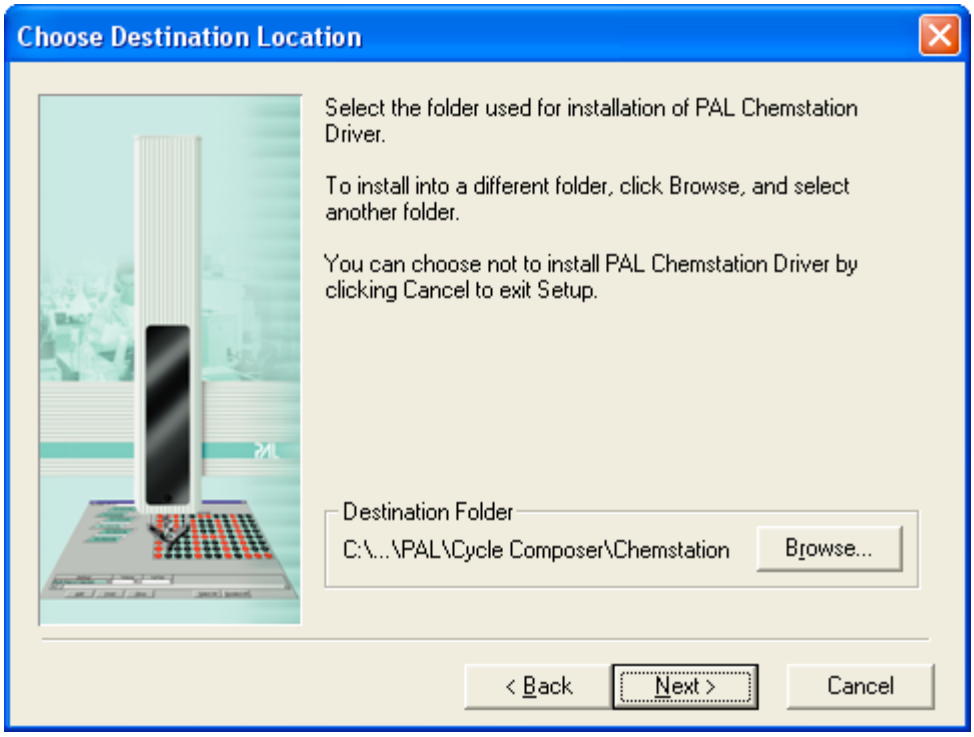
Note:
CTC Analytics advises to check always the read-me file on the Cycle Composer CD for any latest changes or information.

2.2 Installation for GC / HPLC and LC-MSD

Select the folder "*Driver ChemStation 2-1-3*" and double-click the file "*setup.exe*".

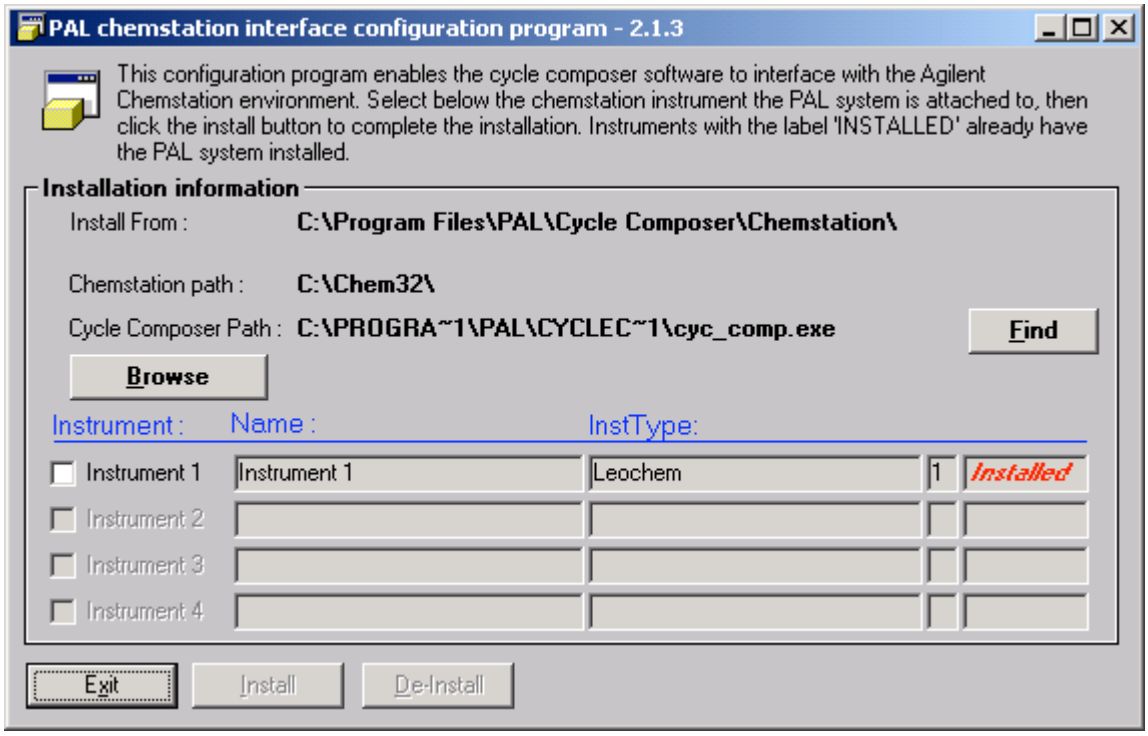


Continue to "*Choose Destination Location*", select the ChemStation Folder.



The installation program analyzes the ChemStation configuration to detect configured instruments. Select the instrument to be used with the PAL Autosampler.

The installation program will automatically create backup copies of all files replaced during the installation process. Path: Program Files\PAL\Cycle Composer\Chemstation\Backup.



If an LC/MSD is configured, only "*Instrument 1*" should be active.
Note that 1100 series LC modules are detected as InstType = 1050.

Enter the correct path for the Cycle Composer software and select the corresponding instrument.

Reboot the computer after the installation of the Agilent ChemStation Driver.

If an 1100 Series autosampler is configured on the LC system, the "*Use Manual Injection*" option (in the "*Method & Run View*" section of the ChemStation) has to be selected when Cycle Composer is launched from the PAL menu.

2.3 Installation for a GC-MSD

This ChemStation version requires a somewhat different installation since this software does not recognize the AddOn interfacing strategy.

The installation program will automatically recognize the installed GC-MSD version, 1701B or C. The corresponding .dll-files will be executed accordingly.

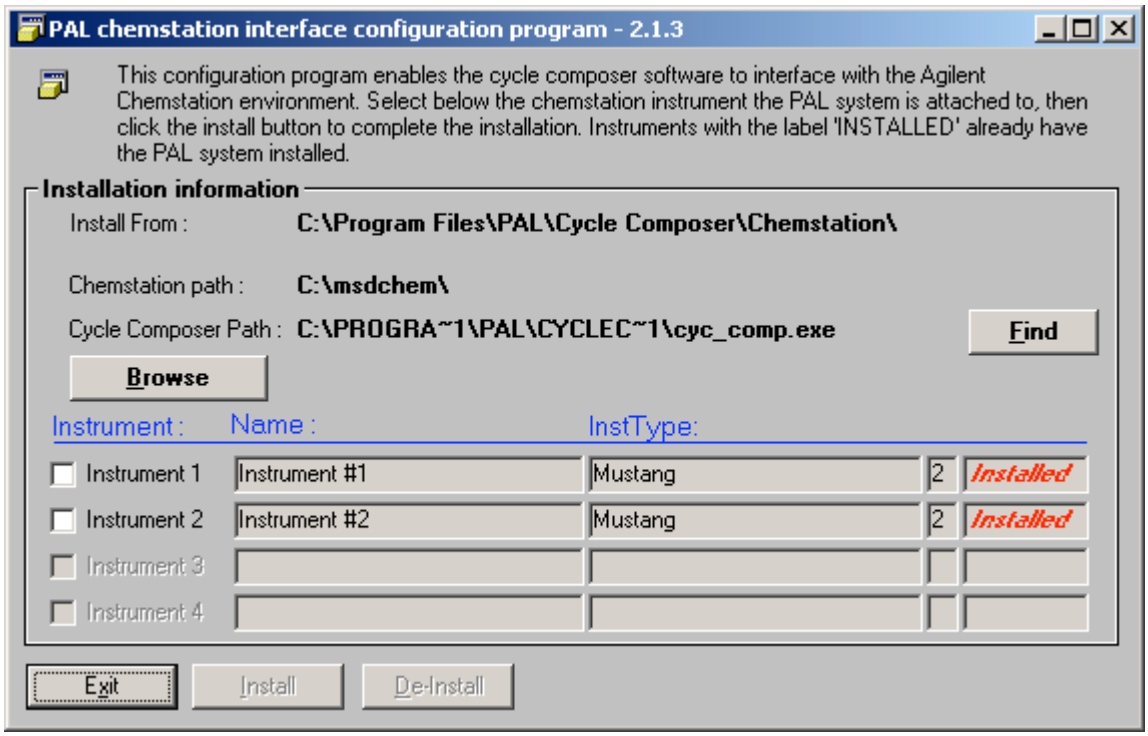
The installation program will modify the standard "*TOPMENU.MAC*". This macro is located in the "*MSEXE*\" directory, right below the main ChemStation sub directory. During installation the original "*TOPMENU.MAC*" macro is copied by the installation program. The location of this file is also in the "*MSEXE*" directory.
The name of the copy is "*TOPMENU.CTC*"

Furthermore the installation will copy two macro files into the "*MSEXE*" directory of the main ChemStation sub directory. The names of these files are "*CTC_INFO.MAC*" and "*CTC_MENU.MAC*".
During the installation process, an Empty ChemStation Sequence File has to be created. This is only required for the ChemStation G1701B.
Details are given below, see chapter 2.3.2.

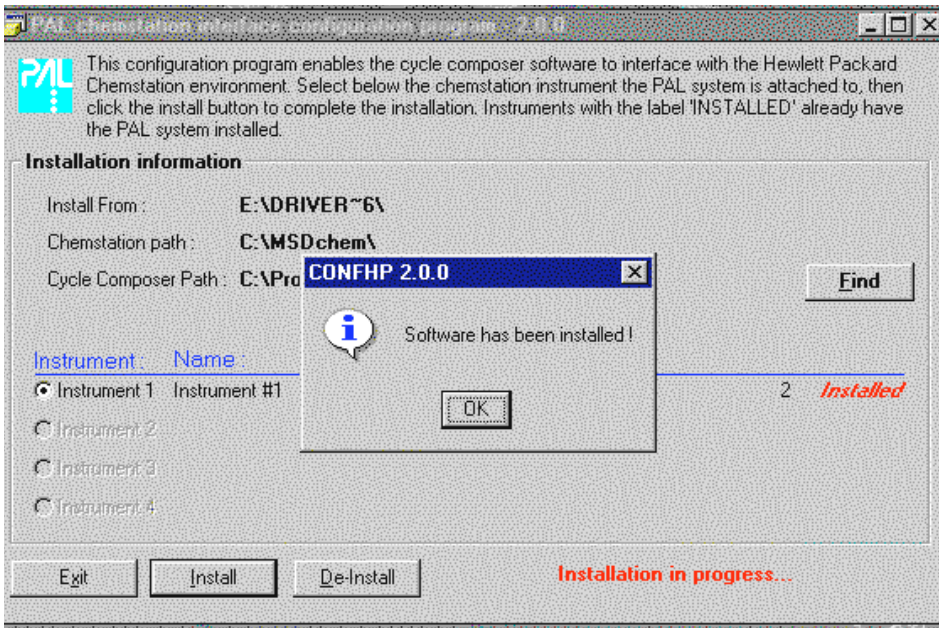
On the Cycle Composer CD select the folder "*Driver ChemStation 2-1-3*" and run "*setup.exe*". This will launch the installation utility which loads the software.

Follow the instructions of the setup utility and check the correct path as shown for ChemStation and Cycle Composer in the figure below.

Select the Instrument to be integrated (only one supported). Select the "*Install*" button.



The installation process is automatically completed. The following message is displayed.



Note:
It is essential to close all programs and re-boot the computer before proceeding

2.3.1 Extra Timer for GC-MSD ChemStation

There are some indications, that the ChemStation sends already a start signal while the report processing is still in progress.

To avoid any possible communication conflict, a special parameter has been built into the driver starting with revision 2.0.4.

Path: HPChem\Core\CTC-CSx.ini

Parameter: ExtraWaitForStart=0 (default : 0 seconds)

In case communication problems are observed, the value of this parameter can be increased.
.

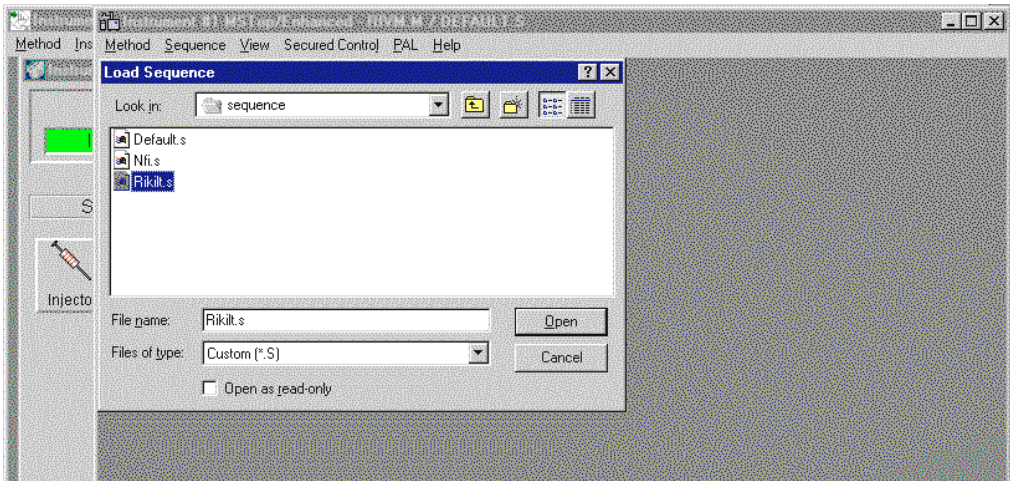
2.3.2 Empty Chemstation Sequence File

The procedure described below to create an empty sequence is only necessary for the ChemStation G1701B. This 16 bit version is used with the MS 5973 with the HPIB communication.

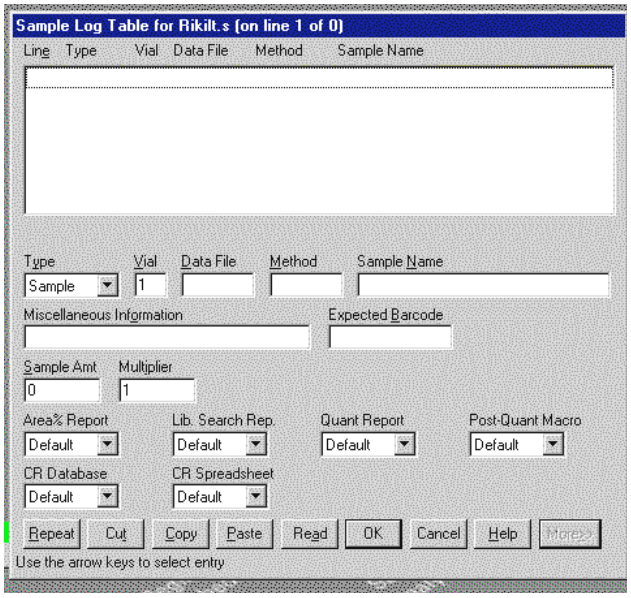
The 32 bit software G1701C is used for the MS 5973 N . For this version and higher the procedure to create the empty sequence file is not needed.

Create an Empty Chemstation Sequence File

The installation program is not able to create an Empty Sequence file, which is necessary for the PAL integration to run properly. The first time the Chemstation is started after the installation of the driver, from the top level menu select "*Sequence / Load*" and open the default sequence template "*Default.s*".

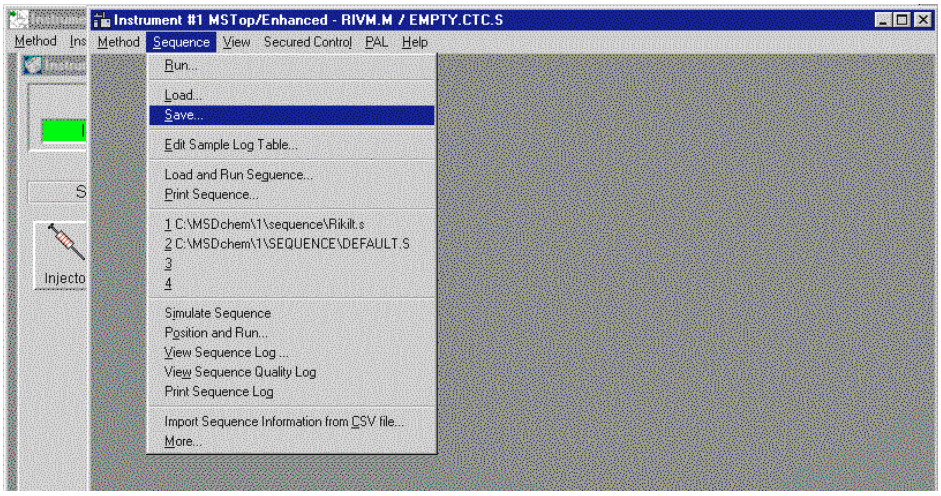


Delete any existing samples in the sequence table using the "*Cut*" button until it is empty as shown below.

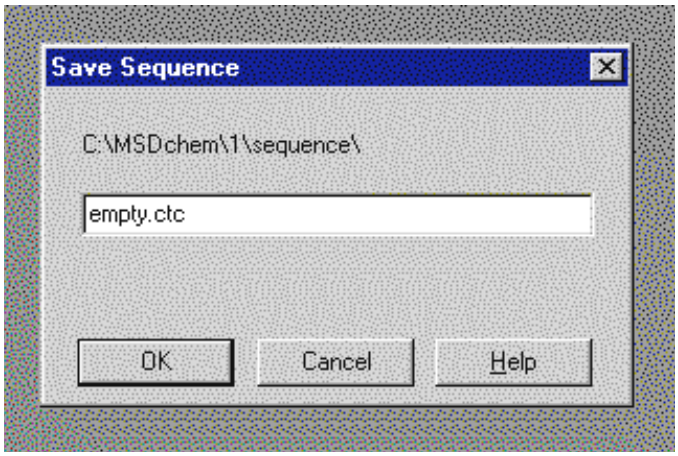


Select "OK" to close the sequence editor

Save the new sequence by selecting the menu “*Sequence / Save*”.

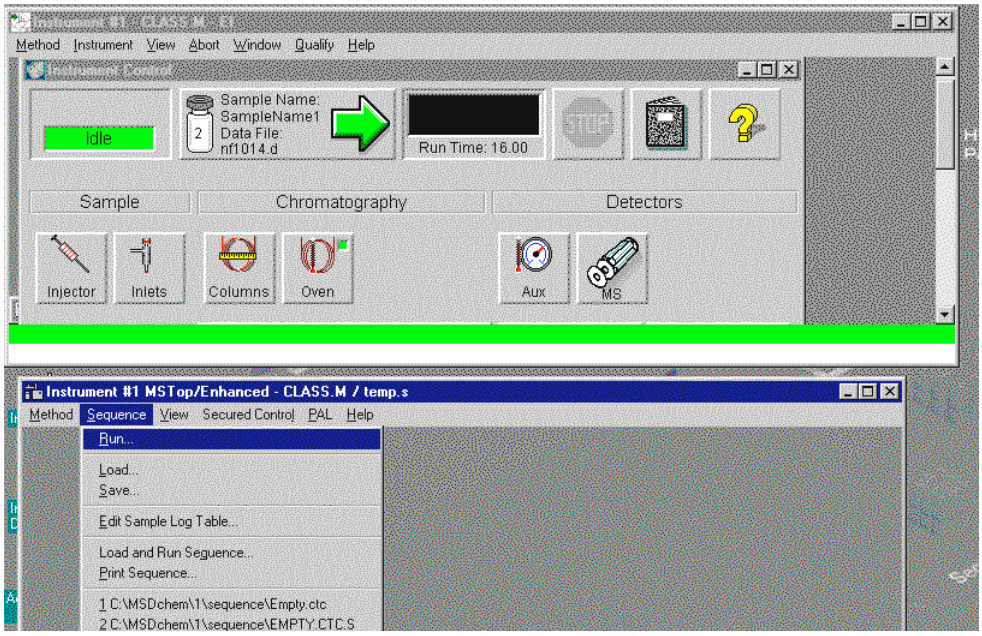


Save the sequence with the name “*Empty.ctc*

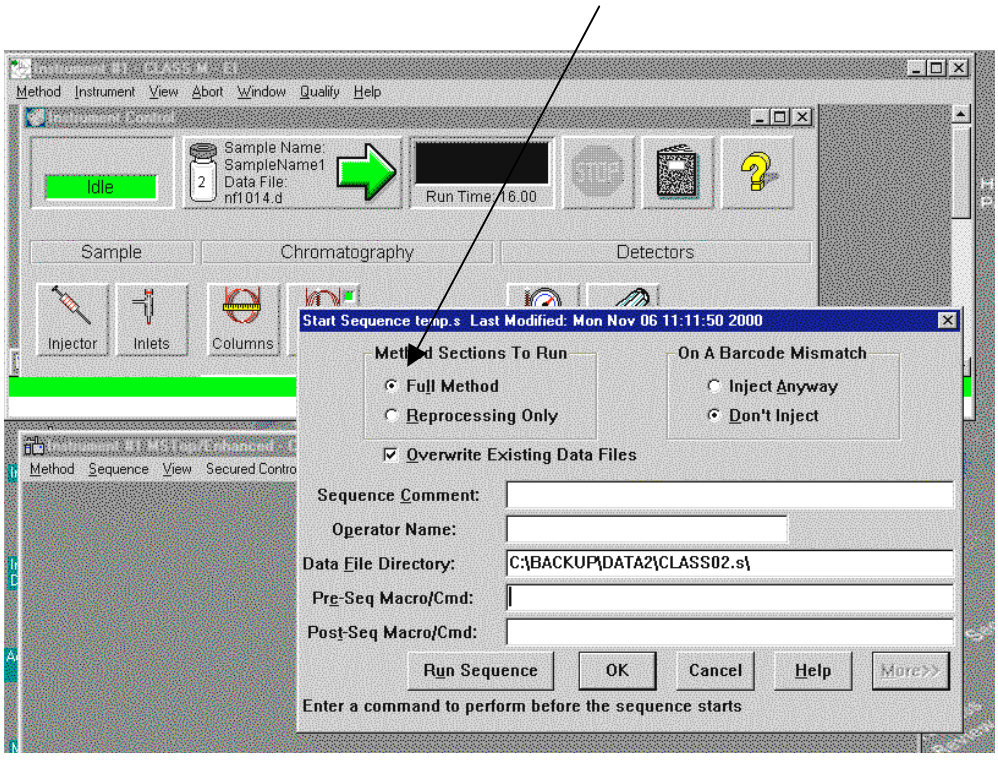


Change the Sequence Default Run Mode

The new sequence will run in “reprocess” mode by default. This mode must be changed to be able to run in “data acquisition mode”.
To do this you must select the menu “*Sequence / Run*”.



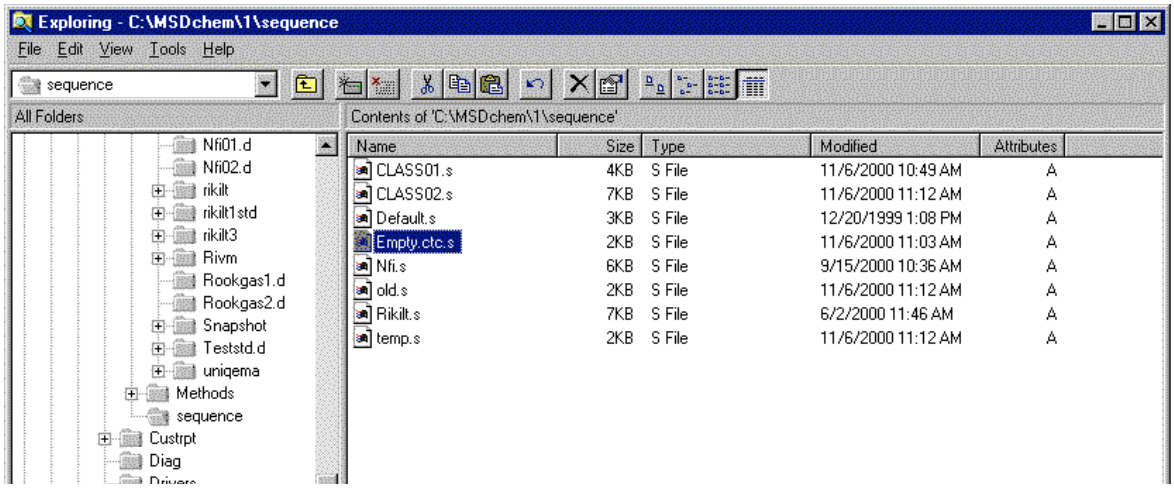
When the run dialogue opens, click the “*Full method*” setting, then click “*OK*”.



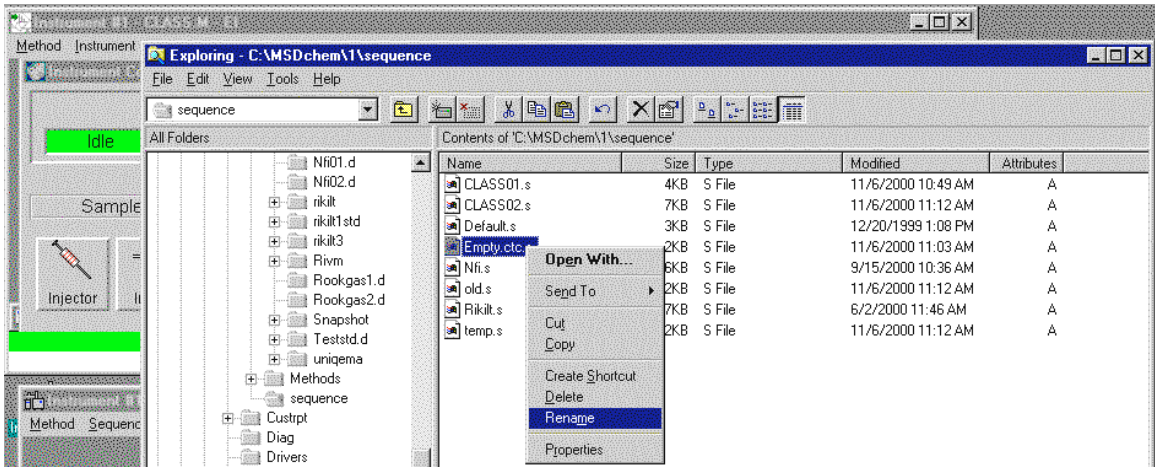
Re-save the method with the same name “*Empty.CTC*”.

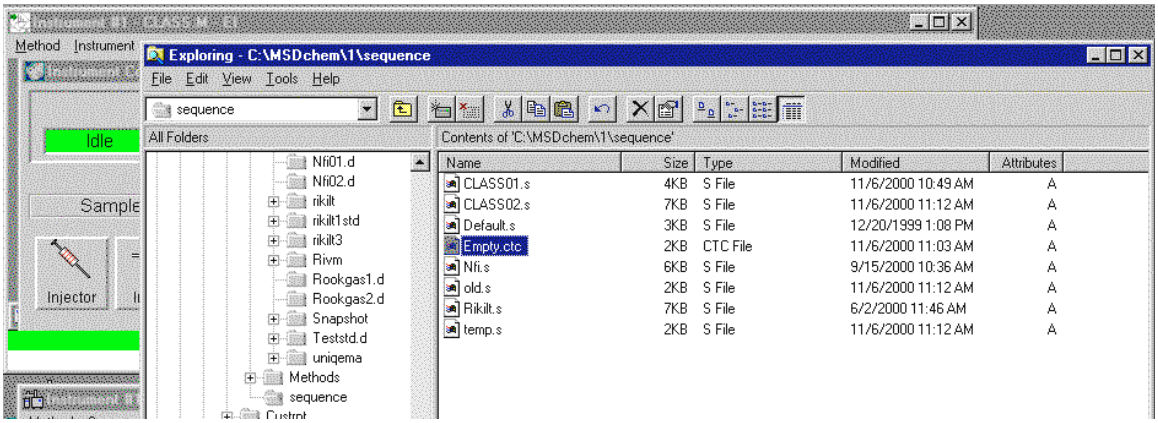
In Windows Explorer, find the "*Empty.CTC.s*" Sequence File.

Right click on the file and select "*rename*"



Rename it to just "*Empty.CTC*". (remove the ".s" extension)





2.4 Files used for Driver Agilent ChemStation - Cycle Composer

File	ChemStation Type	Description
SETUP.exe	For all types	Installation Program to setup the communication between ChemStation and Cycle Composer
STATUS.exe	GC/HPLC/LC-MS	Program to monitor the status of the ChemStation by DDE
PALSEQ.mac	GC/HPLC/LC-MS	Communication Macro
CTC.mcx	GC/HPLC/LC-MS	Communication functions for the driver.
CTC.ini	GC/HPLC/LC-MS	INI-File created during installation
EMPTY.ctc	GC-MSD	Empty Sequence File
TOPMENU.mac	GC-MSD	Modified version of standard file "*Topmenu.mac*", which is replaced and renamed in "*Topmenu.ctc*" during installation.
TOPMENU.ctc	GC-MSD	Renamed standard file "*Topmenu.mac*"
CTC_MENU:mac	GC-MSD	Macro to change the top-menu
CTC_INFO.mac	GC-MSD	Communication Macro
CTC_PRE.mac Note 1)	GC/HPLC/LC-MS	In this macro any other pre-run macro can be included. Listed as the first line in Sequence the macro will be executed.
CTC_POST.mac Note 1)	GC/HPLC/LC-MS	In this macro any other post-run macro can be included. Listed as last line in Sequence the macro will be executed.

Note 1): Do not use the original ChemStation macro possibilities if one macro shall be executed as a pre-/post-run macro. Including the pre-/post-run macro in the ChemStation directly would result in executing the specified macro after every injection.
The pre-/post-run macro shall not be mixed up with the "Keyword Functions". The execution of the Keywords is not possible. See Limitations, Chapter 4.

2.5 Injector Naming / Nomenclature

The injector names should correspond with the nomenclature used in the ChemStation for detecting the front and the rear injector.
In order to be able to select the front or the rear injector, one can use only specific injector descriptions in the local control of a Combi PAL System. For the rear or back injector use: "*Rear*", "*Back*", "*B*" or "*GCInj2*". All other names will automatically refer to the front inlet of the GC.

To insert another injector in the PAL System use the local control terminal and perform the following steps:
Menu / F3 – Setup / Objects / Injector , press F2, "*Insrt Inj*". Give a name to the new injector according to the nomenclature described above. Teach the injector position as described in the Combi PAL manual.

After establishing the serial connection the Cycle Composer will receive all objects from the PAL System. The software will learn at this moment which injectors are configured in the PAL System. With the driver linked to the ChemStation it is ensured that the desired injector will be used.

This nomenclature of naming is important for GC instruments. No special convention or configuration is necessary for HPLC instruments.

2.6 Uninstalling the Cycle Composer Driver for the ChemStation

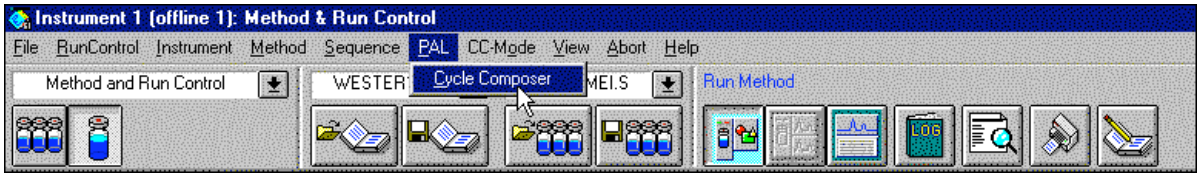
To uninstall the Cycle Composer Driver from the ChemStation use the following procedure:

- Insert the Cycle Composer CD and run the program "*setup.exe*" in the folder "*Driver ChemStation 2.1.3*".
- For GC/LC configurations: remove PALSEQ.MAC
- For GC-MSD configuration:
  - remove EMPTY.CTC
  - rename TOPMENU.CTC back to TOPMENU.MAC

3. Starting Cycle Composer Software in Synchronization with Agilent ChemStation

3.1 Principle of Synchronization

Opening the ChemStation software, a new menu-item **PAL** is added at the top menu of the ChemStation. This menu-item will run a macro which will start the Cycle Composer software.



The Cycle Composer will take control of processing samples. The sequence to run is created by the Cycle Composer including all specific parameters.

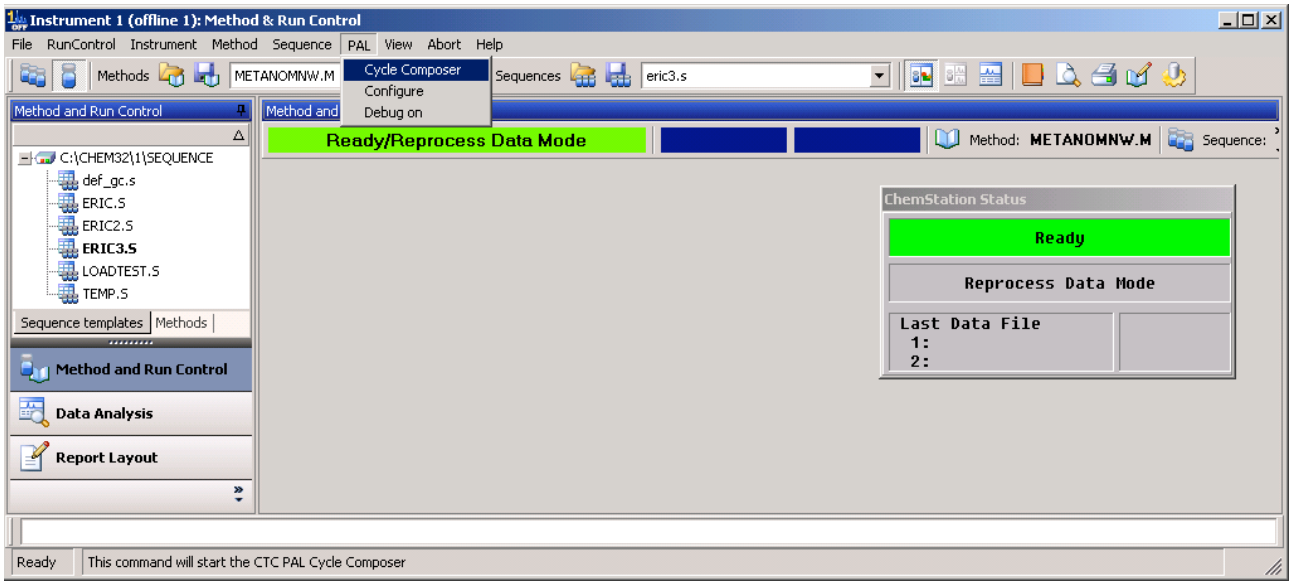
After creating a complete sequence in the Cycle Composer software and starting the sequence using the Start button, the software will check the status of the ChemStation and all information of the current running sample is saved in the .INI file".

If the ChemStation gets into "*Ready-State*" the Cycle Composer will start the processing of the sample list, which contains the ChemStation Method. The macro running the ChemStation will collect the information of the current sample.

The information is attached to the existing sequence and a new sequence-file is created called "*TEMP.s*". This temporarily file is a sequence file for one sample and will be erased and refreshed for every new injection. The complete sequence will be stored in the sequence table which contains all information of all samples and has the same name as the Cycle Composer Sample List.

3.2 Starting the Cycle Composer Software

The PAL Driver installs in the Agilent ChemStation a new menu item, called **PAL**.



Activating the menu "*PAL / Cycle Composer*" opens the Cycle Composer Sample List, with all necessary columns for the ChemStation.

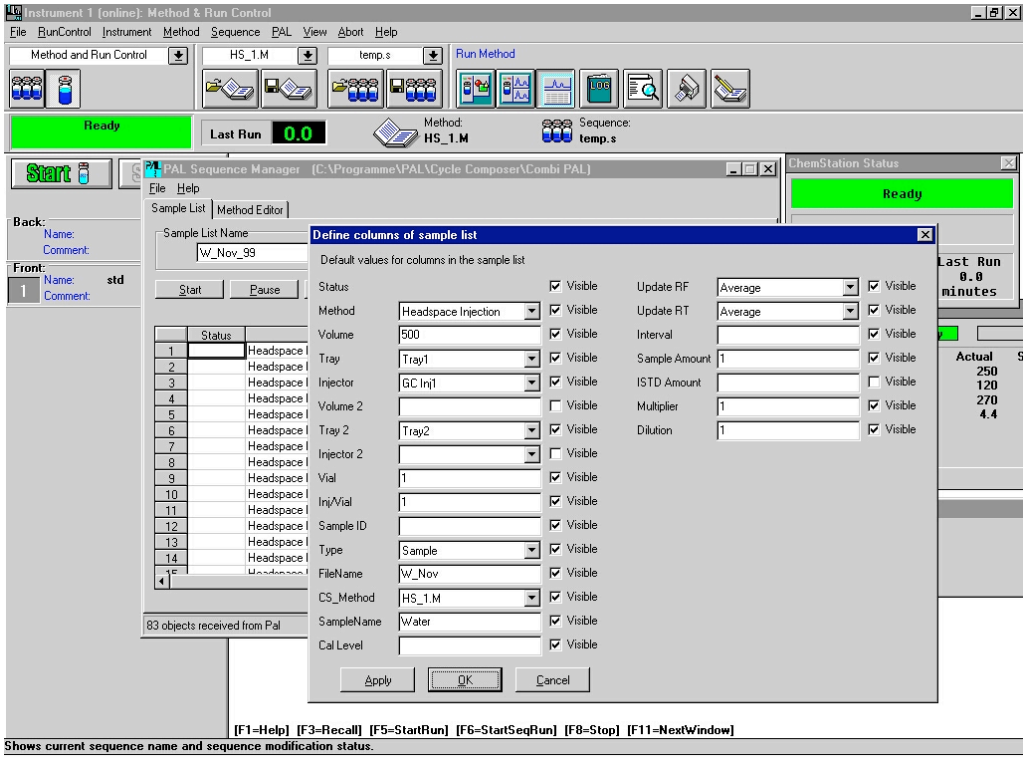
3.3 Creating a Sequence

The Agilent ChemStation specific fields are imported to the existing fields in the Cycle Composer Sample List.

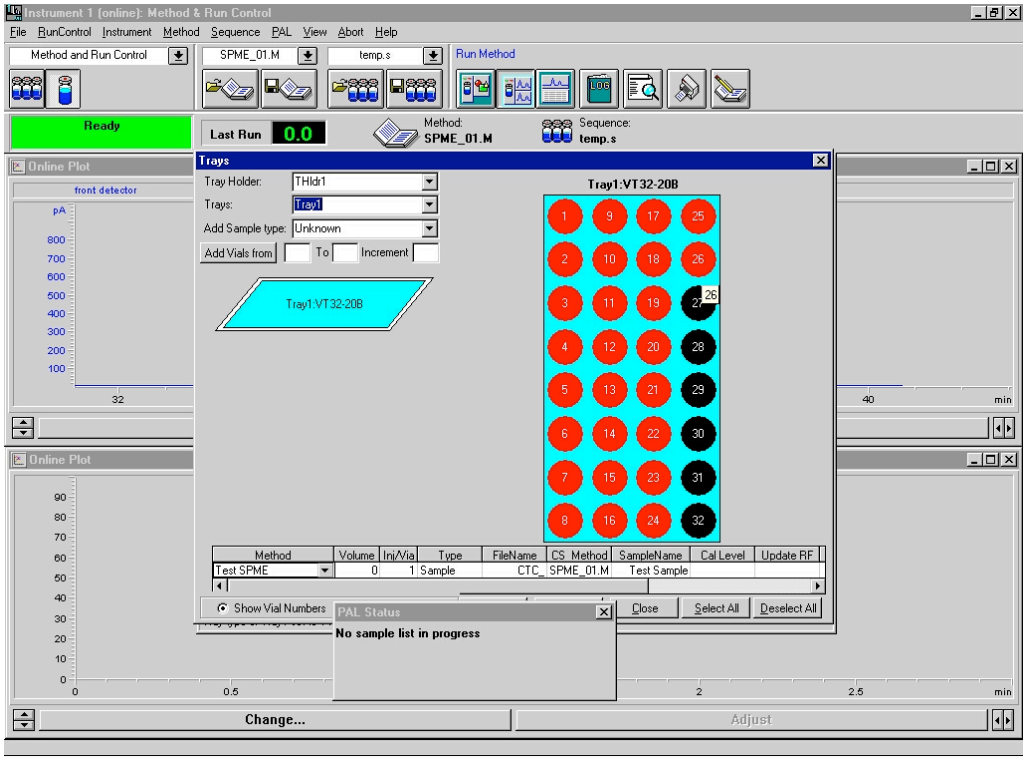
ChemStation specific fields are:

CS-Method	File Name	Sample Name
Update RF	Multiplier	Sample Amount
Update QI	Dilution	Cal Level
Update RT	Interval	ISTD
Type	FIA	

The fields (columns) appearing in the Cycle Composer Sample List can be hidden by unmarking the column name in the File/Option/Format Sample List... -window.



The Cycle Composer software maintains the full functionality. For example the button "*Select Vial*" opens a window for the graphical selection of the vials.



The Cycle Composer Sample List is quickly filled out with the help of the graphical tool. To select the samples for the Sample List, click and drag the mouse over the range of wells or vials to be run. The selected samples will be shown in red. This graphical interface helps to avoid typing errors.

To run a standard (non-FIA) sequence with these samples, select the PAL method, e.g. "*Single Step LC Injection*".
You will also need to specify a file name (5 character prefix + counter), injection volume (Volume), ChemStation method (CS Method), and sample name (SampleNam).

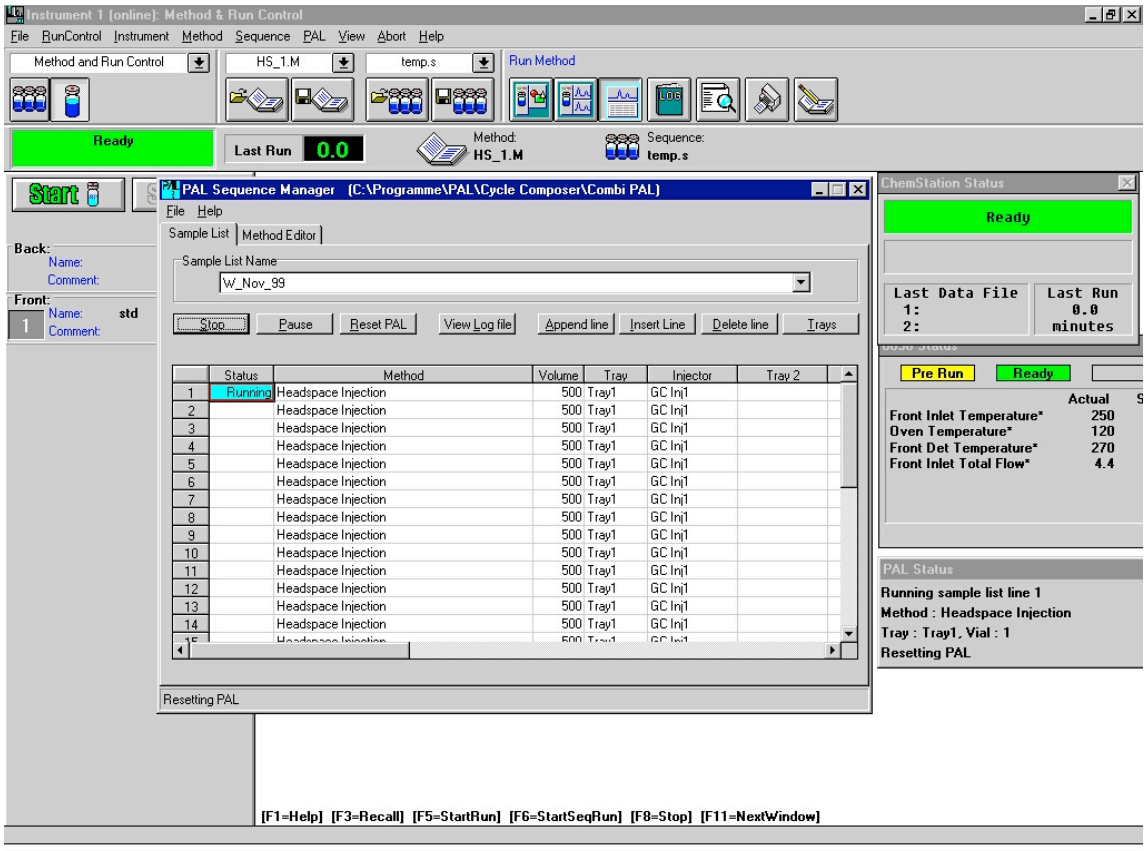
To add the selected samples to the Sample List, select "*Add Vials*". To insert additional vials to the sample list, you may return to the "*Trays*" view to select additional sample positions. You may then use the "*Insert Vials*" selection to add these to the Sample List.

The user has the choice to fill out the filename directly in the column "*Filename*".
Another approach is to specify the constant root of the filename and let the Cycle Composer complete the name with incrementing a 3 digit number, e.g. W_Nov001 ; W_Nov002 ; W_Nov003 , etc..

Note: If the Sample List exceeds 1000 lines, the ChemStation software will run the Sample List as two or more sequences. Data file naming will continue with a 4 character prefix + counter format (i.e. "samp1234.d").

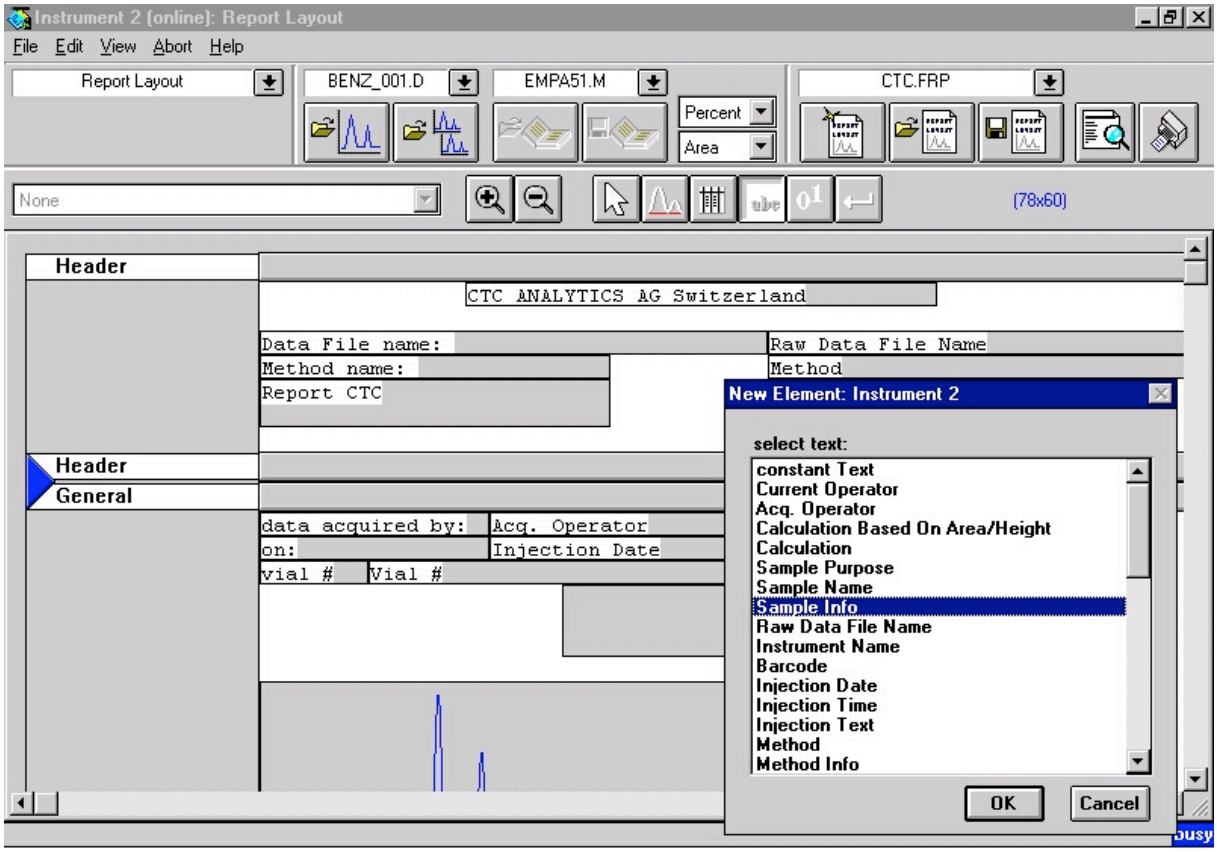
To run the Sample List, be sure the "*Use Manual Injection*" is selected in ChemStation, then select "*Start*" from the Sample List screen.

You must save the Sample List before a sequence can be started. The name is limited to 8 characters for some ChemStation versions. This name will be used to build a ChemStation Sequence Table as the Sample List is run.



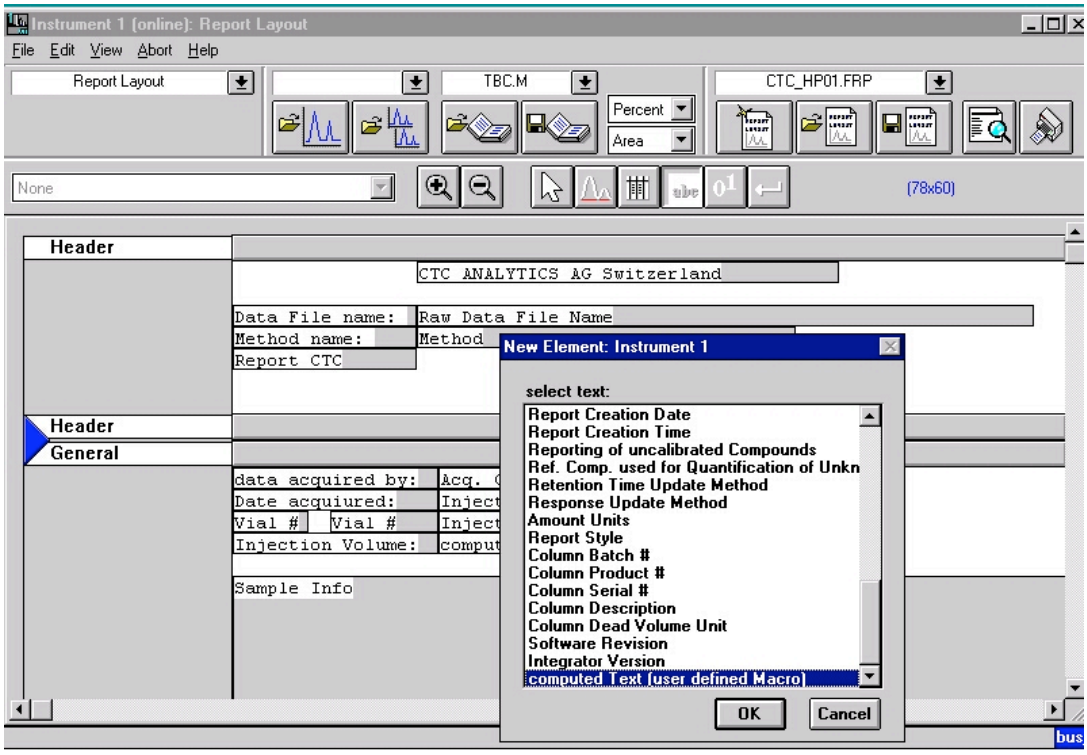
3.4 Customizing a ChemStation Report Template

The Report generator of ChemStation allows the user to customize the report template accordingly to his needs. All ChemStation fields from the sequence are available as usual. The new fields from the Cycle Composer Sample List can be added to the report template by using the "*Sample Info*" (GC/LC/LC-MS) or the "*Miscellaneous Info*" (GC-MSD).

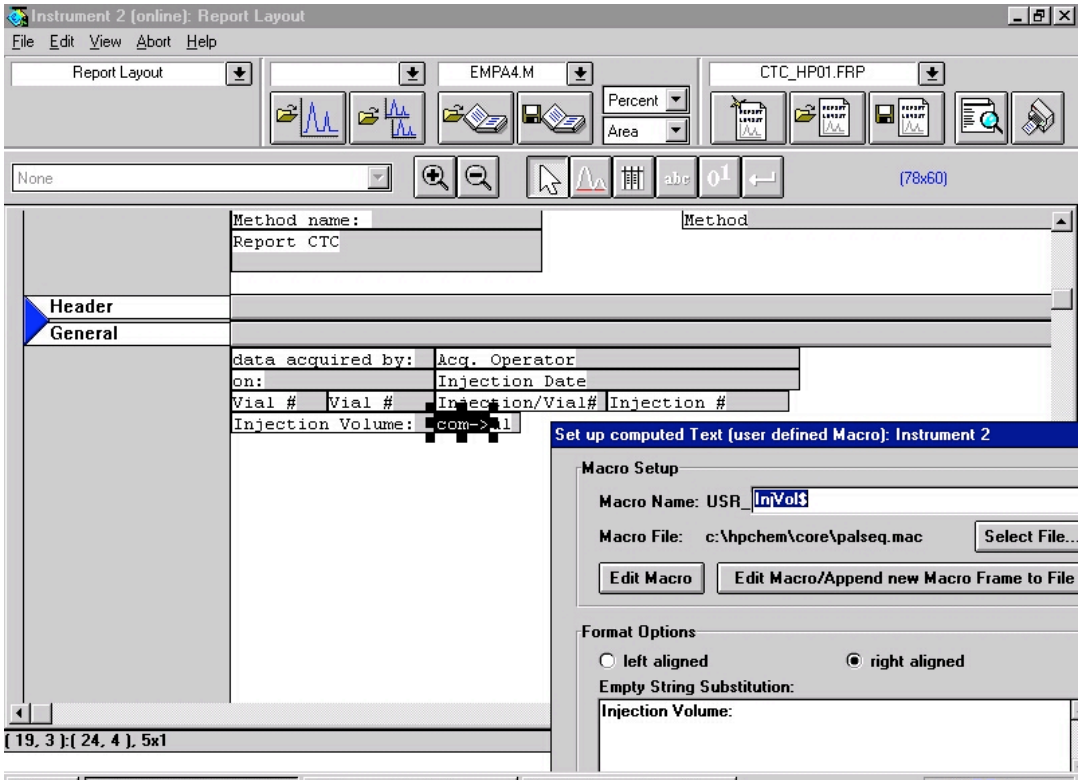


In this field "*Sample Info*" or "*Miscellaneous Info*" all Cycle Composer specific parameters are listed, e.g. Method, Volume, Tray, Sample ID. If the Injection volume is the only parameter to be reported, the function of "*Computed Text*" can be used as described below.

The "*Injection Volume*" is one field of the Sample List and is written directly into the ChemStation Sequence. Since this field is not generated by an Agilent autosampler, it is necessary to retrieve the value by a "*Computed Text*". This allows to print the Injection Volume on the report.

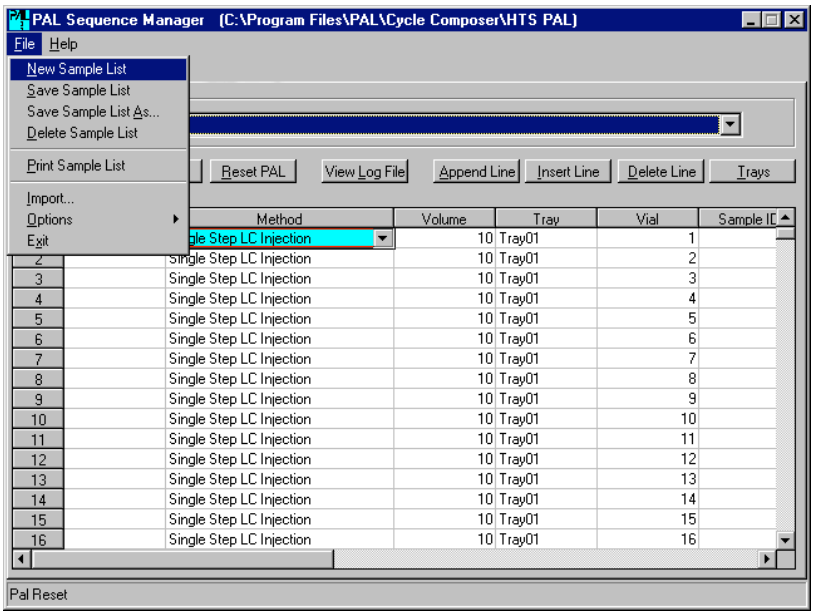


Define the Macro Name as "*InjVol$*", Macro File path as "*c:\hpchem\core\palseq.mac*". The "*Empty String Substitution*" field has no direct effect on the reporting.



3.5 Running a Standard (Non-FIA) Sequence (Sample List)

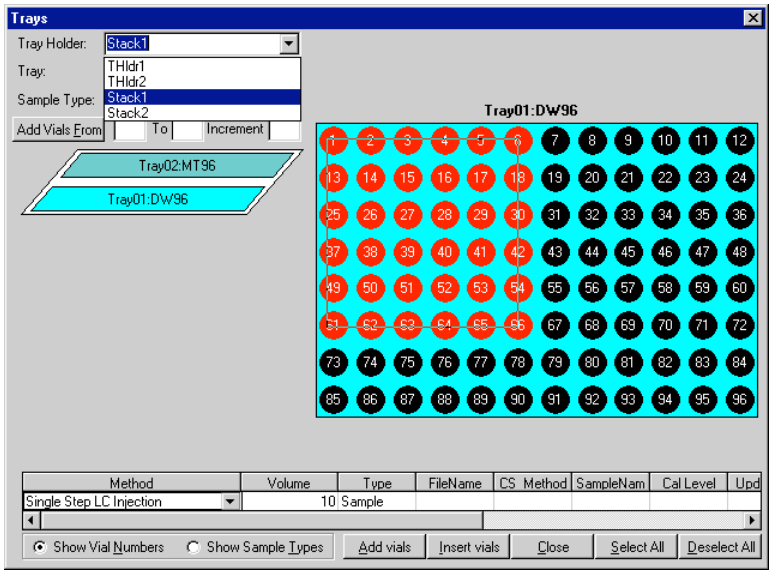
Launch Cycle Composer from ChemStation. This will bring up the PAL Sample List. From this utility, you can build and customize Sample Lists (i.e. sequences or studies) and edit the HTS PAL method parameters. The Cycle Composer Sample List determines the ChemStation method, sample volume, tray and vial positions, etc. that will be run. The Sample List is used to build a ChemStation Sequence Table, which is used to control the LC, GC or MS instruments for data collection and for reprocessing data.



To begin building the Cycle Composer Sample List, select "*New Sample List*" from the File menu. You will be prompted to name the new Sample List. The Sample List name is limited to 8 characters for some ChemStation versions.

To specify the samples that will be run, select the "*Trays*" button. This will bring up a list of the Tray Holders which are configured for the HTS PAL system. The tray(s) for the selected Tray Holder will be displayed on the screen, indicating the tray orientation and well or vial numbers. The sample tray can consist of test tubes, vials or a variety of well plates.

To select the samples for the Sample List, click and drag the mouse over the range of wells or vials to be run. The selected samples will be shown in red.



To run a standard (non-FIA) sequence with these samples, select the PAL method "*Single Step LC Injection*".
You will also need to specify a FileName (5 char. prefix + counter), injection volume (Volume), ChemStation method (CS Method), and sample name (SampleNam).
To add the selected samples to the Sample List, select "*Add Vials*".

Note: If the Sample List exceeds 999 lines, the ChemStation software will run the Sample List as two or more sequences. Data file naming will continue with a 4 char. prefix + counter format (i.e. "*samp1234.d*").

To insert additional vials to the sample list, you may return to the "*Trays*" view to select additional sample positions. You may then use the "*Insert Vials*" selection to add these to the Sample List.

To run the Sample List, be sure the "*Use Manual Injection*" is selected in ChemStation, then select "*Start*" from the Sample List Screen. You must save the Sample List before a sequence can be started. The name is limited to 8 characters. This name will be used to build a ChemStation sequence table as the Sample List is run.

As the Sample List is being run, the Status column will indicate "*Preparing*", "*Running*" or "*Done*".

3.6 Running a FIA Sequence (Sample List)

Setting up a sample list for FIA is very similar to setting up a non-FIA sample list.
Select menu "*PAL / Cycle Composer*" to bring up the Cycle Composer Sample List.
Select "*New Sample List*" from the File menu.

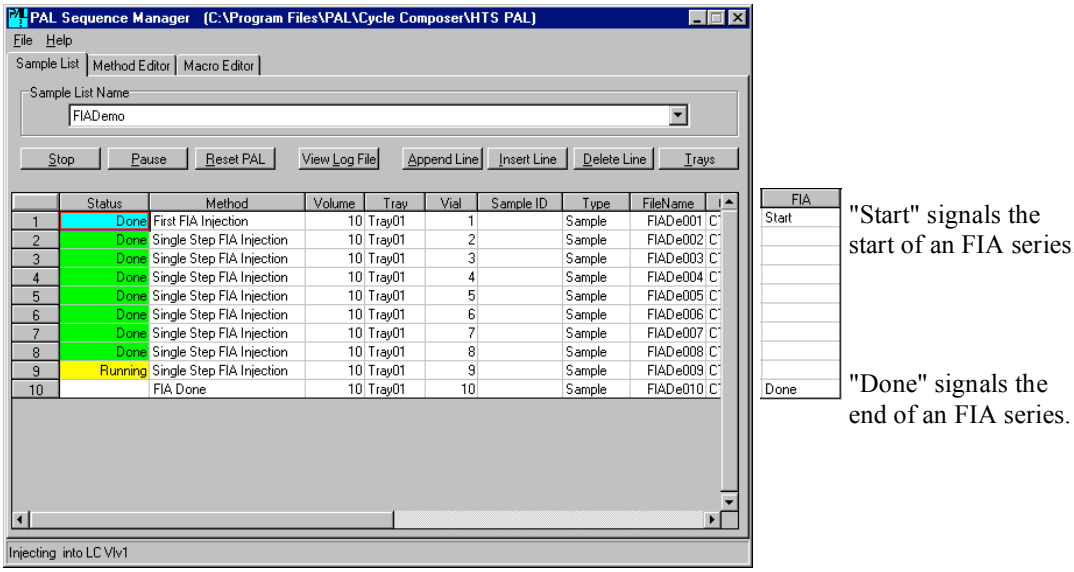
Select the "*Trays*" button to specify the samples that will be run. Specify the tray holder and tray to be used, then click and drag the mouse over the range of wells or vials to be run.
The selected samples will be shown in red.

To create an FIA sequence with these samples, select the PAL method "*Single Step FIA Injection*" from the "*Trays*" method pulldown. Also specify the injection volume (Volume), FileName (5 char. prefix + counter), ChemStation method (CS Method), and sample name (SampleNam). Select the "*Add Vials*" button to add the selected samples to the Sample List. Close the sample selection window to return to the Sample List.

Change the Method of the first line of the FIA series to "*First FIA Injection*" and select "*Start*" in the FIA column. This is generally the last column in the Sample List.

Note: If the FIA column is not visible in the Sample List, use the menu "*File/Options/Format Sample List*…". Activate the FIA field.

Change the Method of the last line of the FIA series to "*FIA Done*" and select "*Done*" in the FIA column. At this point, the Sample List should look something like the figure bellow.

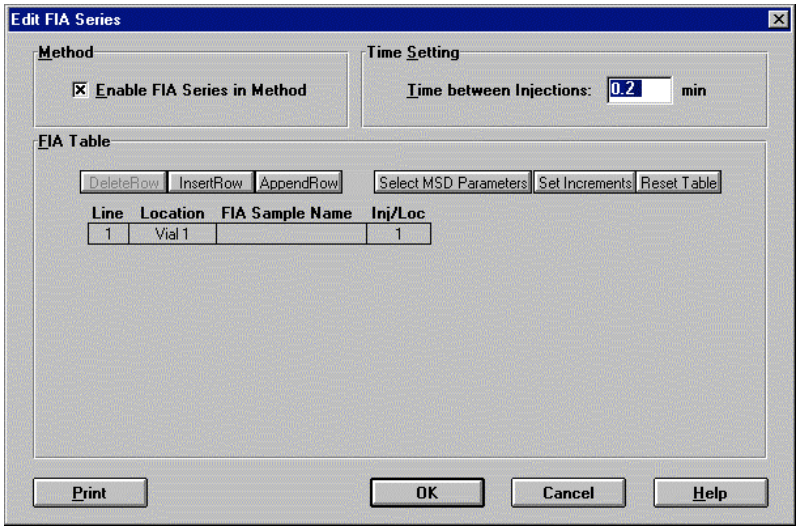


Although each injection is shown as a separate line in the Sample List and the field FileName is also incremented, the data is ACTUALLY collected to a single data file with the filename taken from the first line of the FIA sample list.

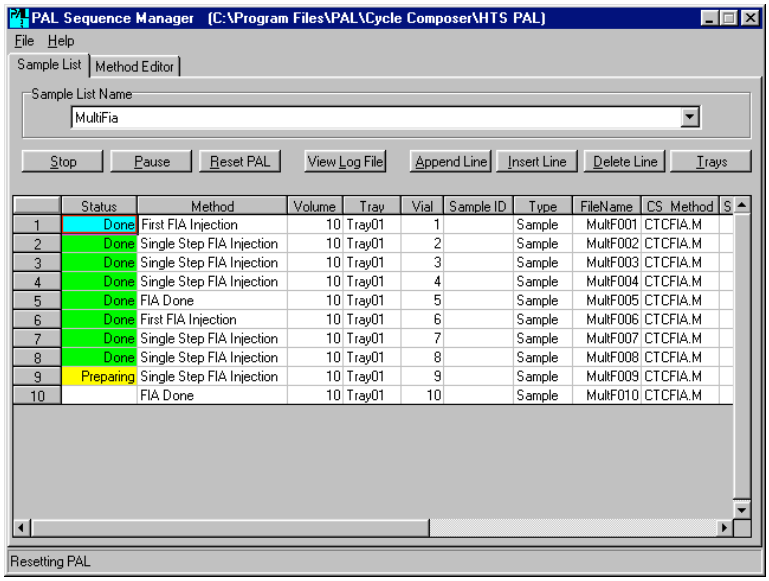
In addition to using the "*First FIA Injection*" method, the first line of the FIA Sample List must also contain a "*Start*" indicator in the FIA column. This signals the PAL software to begin an FIA series. Likewise, the "*FIA Done*" method and "*Done*" indicator in the FIA column signal the end.

Notes:

a. The ChemStation method **MUST** be a FIA method. The ChemStation FIA table is ignored except for the time between injections. This is generally set to the shortest allowable time, 0.2 min.
b. If the Sample List exceeds 1000 lines, the ChemStation software will run the Sample List as two or more sequences. Data file naming will continue with a 4 char. prefix + counter format (i.e. "samp1234.d")



A multiple FIA Series sequence can also be created in the Sample List by adding additional "*First FIA Injection*" and "*Start*" lines.
This is functionally equivalent to the "*Run Multiple FIA methods*" feature in ChemStation. Each FIA series also requires the "*FIA Done*" method and "*Done*" selection in the FIA column to end the FIA series.



"Start" and "Done" indicators are required for each FIA series in the Sample List.

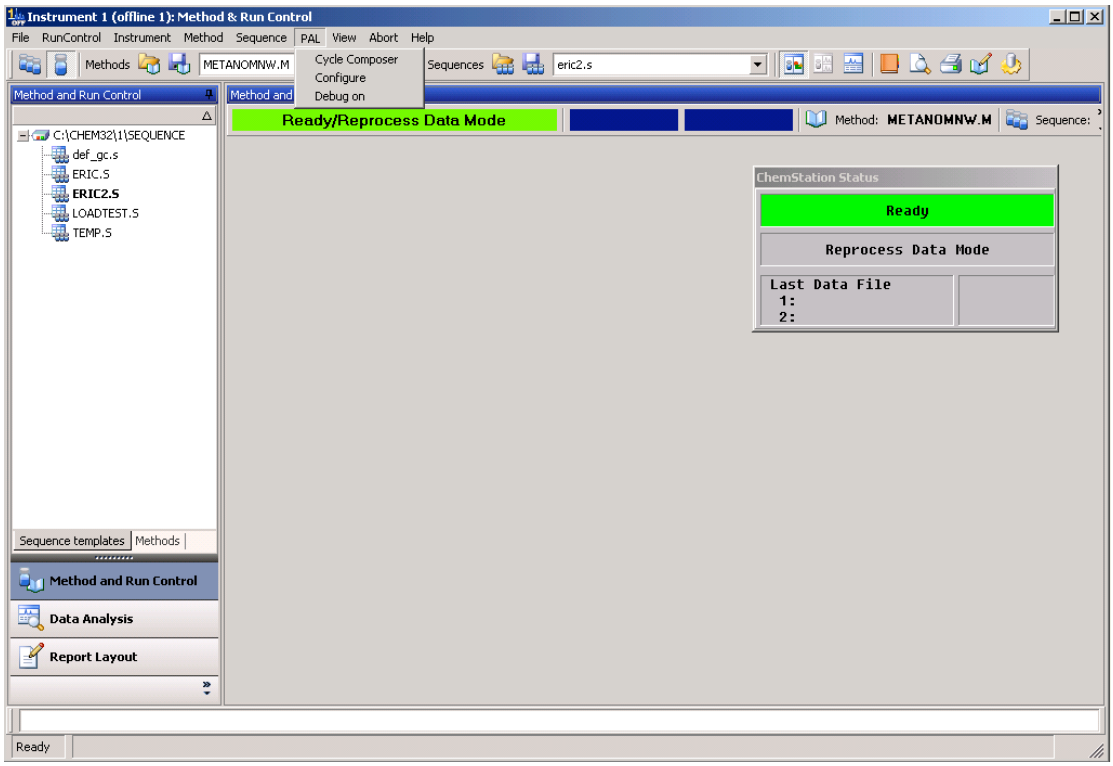
To run the FIA Series Sample List, select the "*Start*" button of the Sample List Screen. You will be prompted to set the Pump Off time to "*Off*" if it currently has some time value. Select "*Ok*". This prevents a stop signal from being generated during the FIA series.

Note: When the sample list is running, the "*Start*" button changes to "*Stop*".

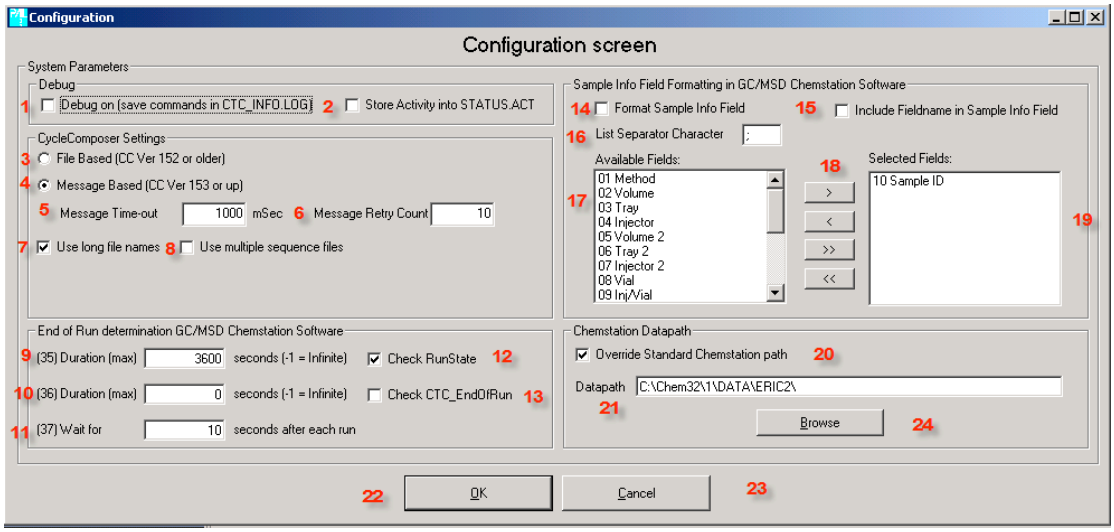
3.7 Configuring the Chemstation interface

From the ChemStation menu it is now possible to run the configuration dialog for the interface between Cycle Composer and ChemStation.

Two menu items inside the Chemstation PAL menu are available, the "*Configure*" and the "*Debug*" menu.



The Configure menu will display following window:



The meaning of the individual items is explained by the number:

1) Set the debug mode when the ChemStation software is started. When enabled a file called CTC_INFO.LOG is created in the msexe or core directory right beneath the chemstation directory.

2) Enabled or disables the creation of a file called STATUS.ACT. This file contains the steps in time taken by the interface. The numbers in this file refer directly to the secondary tab steps when in debug mode.

3) When an older version of the Cycle Composer is installed (older then 1.5.2) the messaging mechanism of windows is not supported yet. So commands between the two modules (Status.exe and Cycle Composer) are exchanged by means of files. In some rare occasions this might lead to file sharing violations and should only be used when the Cycle Composer 1.5.2 or newer is not at hand.

4) Message based command exchange is enabled with this setting, see explanation for item 3

5) When Item 4 is enabled this setting is used to control the time-out between the two modules in case of problems.

6) When Item 4 is enabled this parameter sets the number of retries used between the two modules to exchange messages.

7) This setting will enable the use of long filenames. The maximum length is then depending on the maximum length allowed inside the chemstation version.
Warning: Older versions of ChemStation might not support this setting.

8) This setting is used to split up sequence files when they become too long (more then 1000 entries for most chemstation versions). The interface will then split up the sequence files created in the Cycle Composer in sets of 1000 entries. The name will be adjusted for the last digit to become a counter.

9) This parameter sets the maximum time used to determine the end of a run when item 12 is enabled. So should the runstate parameter of the chemstation not change to the proper status the interface will automatically stop once this maximum time-out value is reached (timer starts together with the run-start!!! So take in account the normal time of a run)

10) This parameter sets the maximum time used to determine the end of macro time for setting the CTC_EndRun parameter. If this parameter is used it is up to the post-run macro to set the CTC_EndRun to 1 in order to signal all actions in the post-run macro are finished. This mechanism is used to create an extra wait time for the next injection when the post-run activities are very time consuming and it is not desired that the next run is started already when post-run activities are still going on.

11) This will set extra wait time after each run.

12) This will enable that the interface keeps checking the runstate parameter of the ChemStation in order to wait for the next run to be started. In some cases the ChemStation runstate parameter in not always accurate and can cause trouble in the interface. If the parameter is not used the interface will always prepare the next run while the actual run is started. The interface will wait in the pre-run phase until the actual run is completed.

13) This will enable the use of a macro parameter to signal readiness of the post-run macro's. If set the post-run macro should contain a statement like this:

    CTC_EndRun = 1

    Should this line be missing in the post-run macro, the interface will wait for the maximum time set in item 9 before continuing the next run.

14) With this setting the interface can perform formatting of the sample-info field based on the settings in items 15-19

15) When selected the fieldnames are also put into the sample-info field. The format is like : method=default.mth

16) This parameters controls the separator character to be used inside the sample-info field for separating the individual entries.

17) This listbox contains all available items from the sequence which can be put inside the sample-info field.

18) Command buttons which enable the user to move fields from the available listbox to the selected listbox:
    - > Add the selected fields(s) inside the available fields box to the selected fields box
    - < Remove the selected fields(s) inside the selected fields box to the available fields box
    - >> Add all available fields to the selected fields box
    - << Remove all fields from the selected fields box to the available fields box

19) This box contains all the selected fields which will be put inside the sample-info field when a run is started. The sample-info field however is very limited and care should be taken which fields are put inside the sample-info field. For the GC-MSD version the size of this field is only 40 characters.

20) This setting will enable the user to override the data path as set by the ChemStation for storing the data files. In the latest releases of the chemstation a nasty bug is present. When a run is aborted, the datapath last selected becomes the base datapath for the next to follow runs resulting in data being stored in the wrong location. In order to prevent this from happening a feature has been created for which the interface will set the default datapath each time a run is started from the Cycle Composer to the datapath as set in the configuration dialog in item 21.

21) This parameter contains the datapath to be used when parameter 20 is enabled. If the path is non existent, the interface will try to create the full path as set here. This will only function if the user has enough privileges for the selected path.

22) Use this button to store the modified configuration.

23) Use this button to return to the original configuration before making any modifications.

24) Use this button to show an explorer style dialog to select a datapath for item 21.

4. Limitations

The following limitations are known at the level as described in this Installation Guide:

1. Some versions of the ChemStation do not allow a file name longer than 8 Characters. This is valid for the run files as well as for the Sample List.

2. With every injection a temporary file is created, called Temp.s. Using this concept, it is not possible to make multiple injections from the same vial. The run file will be overwritten for each sample and only the latest file is stored. (Sequence "*Temp.s*").

3. For GC Instruments it is not possible to use the "*Dual Injection Mode*".

4. Calculation with the so-called Bracket-Mode is not active.

5. In the GC-MSD version it is not possible to select a sample of a user defined-type or a "Keyword-Sample". These values are not loaded with the PAL Driver Macro.

6. Only one Cycle Composer Software can be installed on a workstation. Therefore the control of several Agilent Instruments with one workstation is not possible.

7. The HPLC System Model 1090 is supported with this version of the driver. Limitations have to be made, that the highest upgrade level to hardware as well as software has to be implemented.

8. The ChemStation Version "Cerity" is not supported.

PAL Driver for ThermoFinnigan Xcalibur Data System

Installation Guide

Software Revision 1.5.6

Printing History

Preliminary Installation Guide	October 1999	Software Revision 1.1
Edition 1	December 1999	Software Revision 1.2
Edition 2	May 2001	Software Revision 1.3
Edition 3	July 2001	Software Revision 1.3.1

Release History

Software Revision 1.1	Original Driver for Xcalibur Software.
Software Revision 1.2	Adaptation to Xcalibur Revision 1.1
Software Revision 1.3	Adaptation to Xcalibur Revision 1.2 - Barcode Reader is supported - Syringes with volume larger than 1000 µl are supported - Open Access is supported
Software Revision 1.3.1	Problems with the installation routine (registry) are solved.

Table of Contents:

1. Requirements **67**

1.1 Software Requirements 67

1.2 Workstation Requirements 67

1.3 Requirements for the PAL System 67

1.4 Synchronization Requirements for the PAL System and the ThermoQuest Instrument 67

2. Installation Procedure **68**

3. Using the Xcalibur Software in Combination with Cycle Composer Software **69**

3.1 Instrument Configuration 69

3.2 Instrument Setup 71

3.3 Sequence Setup 73

3.4 Starting a Sequence 76

PAL Driver for Xcalibur Data System

1. Requirements

1.1 Software Requirements

- Xcalibur Software Revision Level 1.2
- Xcalibur Patch # 9537
- Cycle Composer 1.5

The Xcalibur Patch # 9537 is a correction to the ThermoFinnigan Xcalibur Software and has to be requested at ThermoFinnigan.
The Patch is needed to support the Barcode Reader and the scaling in the window "*Real Plot*" is corrected also.

1.2 Workstation Requirements

The Hardware requirements are given by the ThermoFinnigan Xcalibur Data System.
Consult the Xcalibur Manual or a representive of ThermoFinnigan.

1.3 Requirements for the PAL System

The PAL Driver for Xcalibur can communicate with the following Firmware levels of the PAL System:

- Combi PAL 2.2.0 or higher
- GC PAL 2.2.0 or higher
- HTS PAL 2.2.0 or higher
- HTC PAL 2.2.0 or higher
- LC PAL 2.2.0 or higher

1.4 Synchronization Requirements for the PAL System and the ThermoFinnigan Instrument

The synchronization of start/stop/ready signal between the PAL System and the ThermoFinnigan Xcalibur Workstation is done via serial connection. Use the PAL connector SER1 and any serial connector at the workstation.

The PAL System is the Starting Device for the combined system.

The setup for the PAL synchronization signal has been pre-configured by the factory with the setting of the synchronization signal Start = "*immediat*".
Do **NOT** change this value if working in combination with Xcalibur.

Note: In the CTC manual it is mentioned that the Start signal shall be changed from "*immediat"* to "*TTL-In1*". This is valid for a stand alone situation but not working in combination with Xcalibur.

If the PAL System has been used already as a standalone unit it is necessary to change back the Sync Signal settings using the local terminal as follows:

Path: Menu / Setup / Objects / Sync Signals / Start

2. Installation Procedure

Order of Installation:

1. Xcalibur Software 1.2
2. Xcalibur Patch # 9537
3. Cycle Composer 1.5.4
4. PAL Driver for Xcalibur 1.5.6

To setup the communication between Xcalibur and the Cycle Composer, it is necessary that both programs are installed on the workstation.

It is advisable to test both software individually. If both programs are working satisfactory the installation of the PAL Driver for Xcalibur can be made.

Insert the Cycle Composer CD and navigate to the folder "*Driver Xcalibur 1-5-6*". Double-click the program "*PALVI 1-5-6 Installation.exe*" to start installation.

Follow the dialog and enter the correct path for Xcalibur and for Cycle Composer.

Restart the computer after the successful installation.

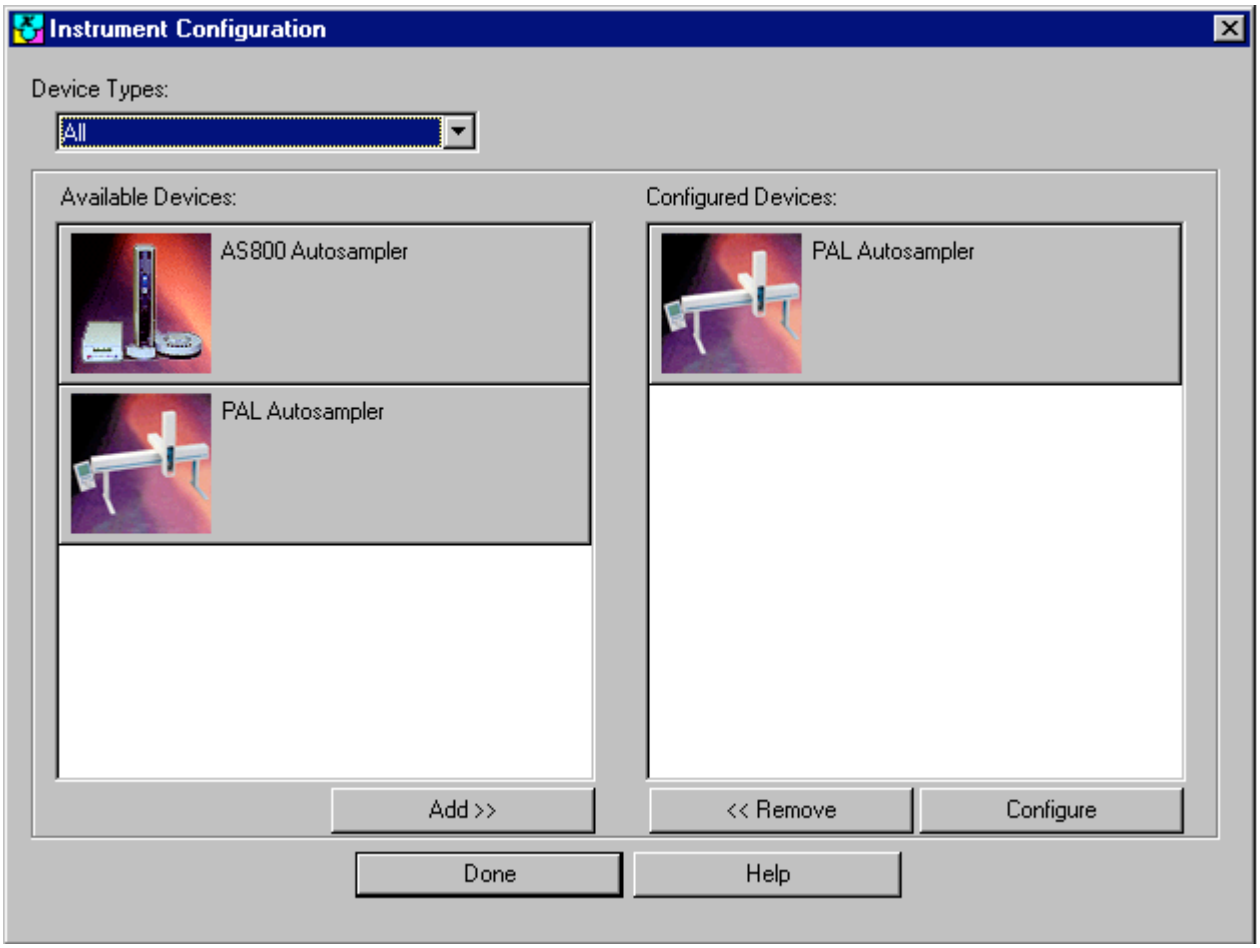
Note:
CTC Analytics advises to check always the read-me file on the Cycle Composer CD for any latest changes or information.

3. Using the Xcalibur Software in Combination with Cycle Composer Software

In this guideline only the two sections “Instrument Setup” and “Sequence Setup” are covered. These sections are directly related to the PAL System. How to use the other Xcalibur sections is outlined in the corresponding manual from ThermoFinnigan.

3.1 Instrument Configuration

Start the program from the desktop Icon “*Instrument Configuration”.*
Select the Icon “*PAL Autosampler*” from the “*Available Devices*” and drag-and-drop it into the page “*Configured Devices*”

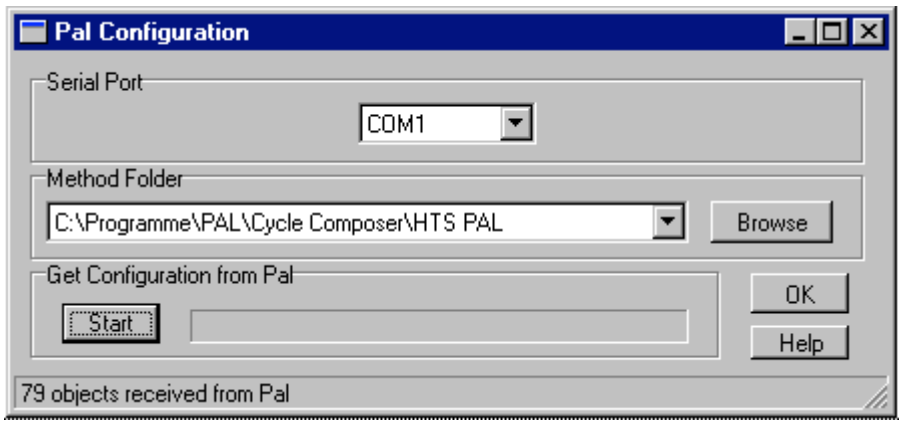


Activate the Icon "*PAL Autosampler*" in the field "*Configured Devices*" and click on the button "*Configure*" and follow the steps:

- Specify the corresponding *Serial Port*, e. g. COM1

- Select the *Method Folder*,
  e. g. C:\Program Files\ PAL\Cycle Composer\HTS PAL

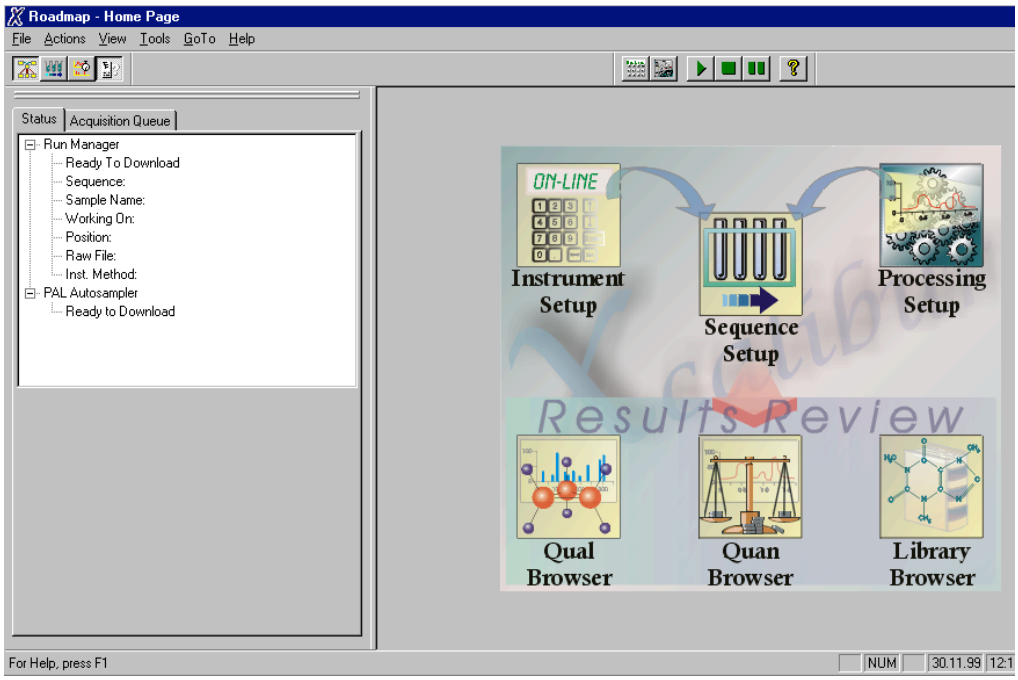
- *Get Configuration from PAL*, click the *Start* button.
  The serial connection will be established and the software will receive the configuration from the PAL System.
  After the successful upload one will get the message:
  "*XX objects received from the PAL*.



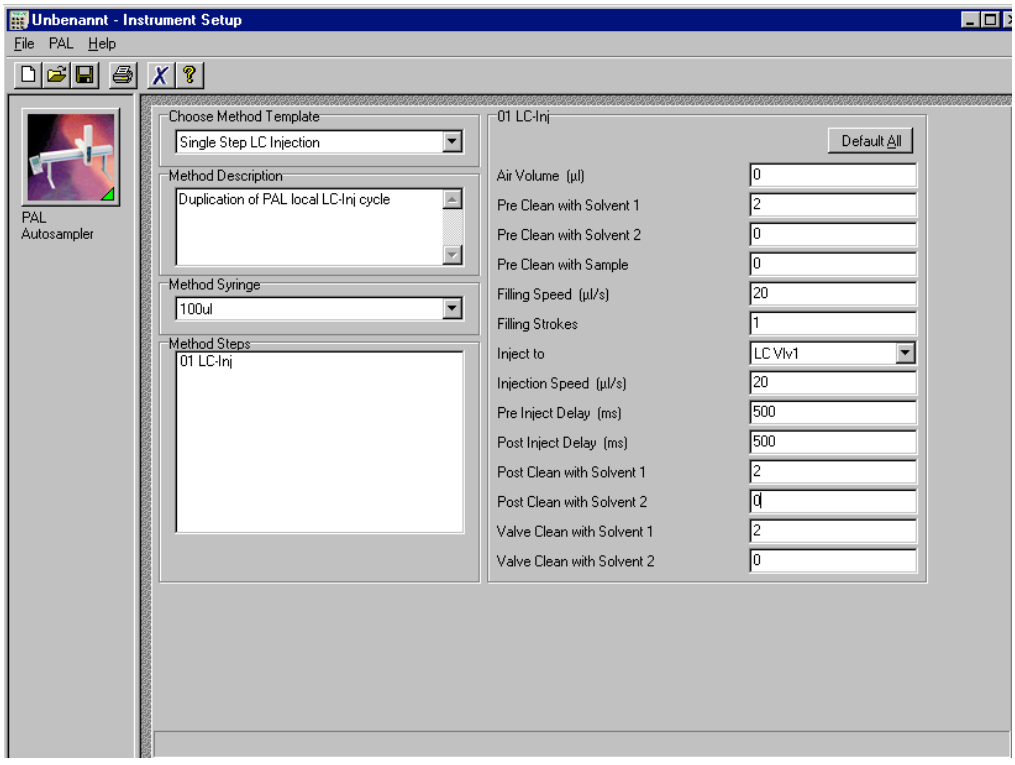
Close the section "*Instrument Configuration*".

3.2 Instrument Setup

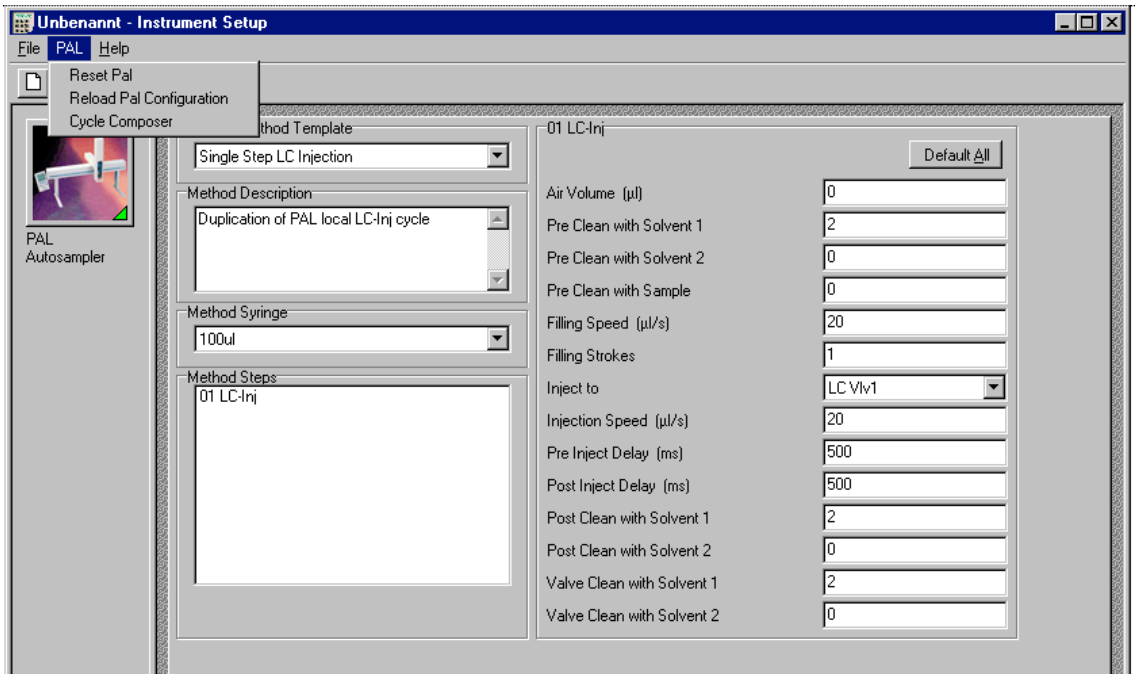
Start the program from the desktop Icon “*Xcalibur*”.



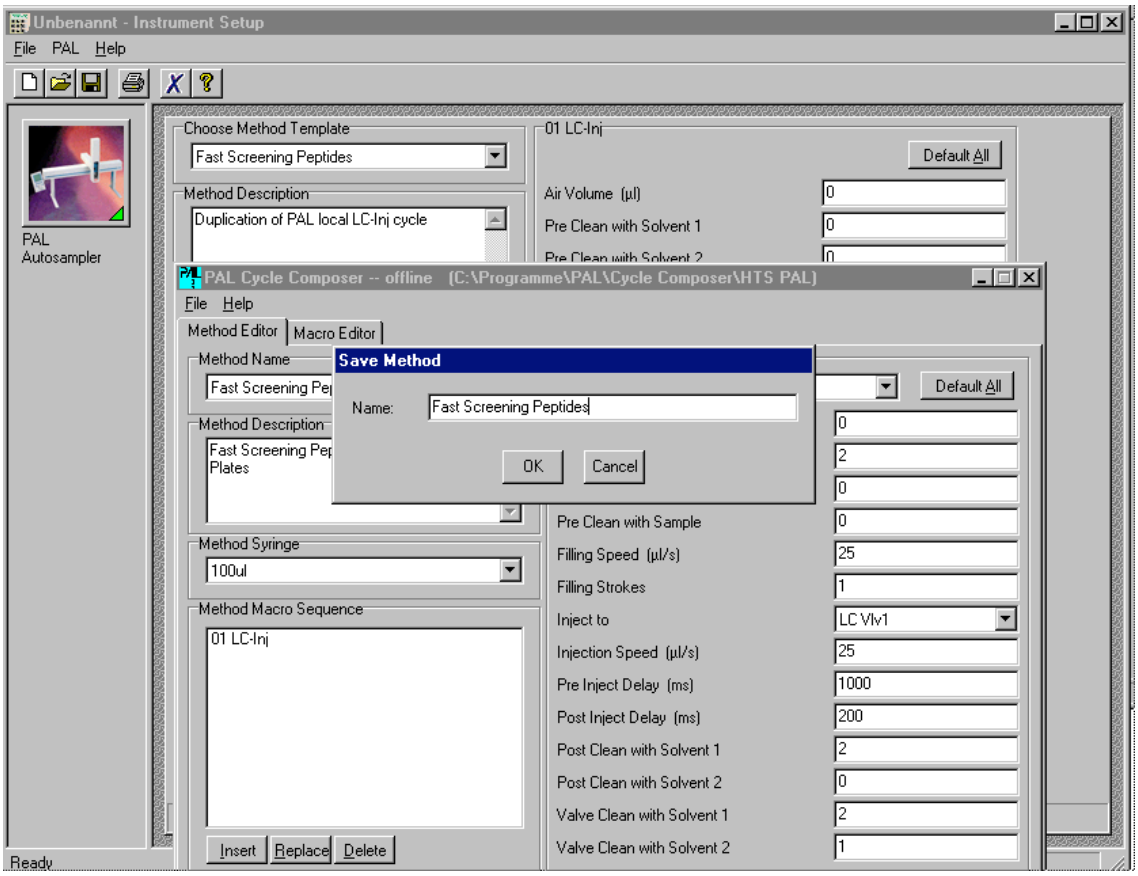
Choose the section “*Instrument Setup*”. As a difference to the standalone Cycle Composer software, the user will get a Method Template.



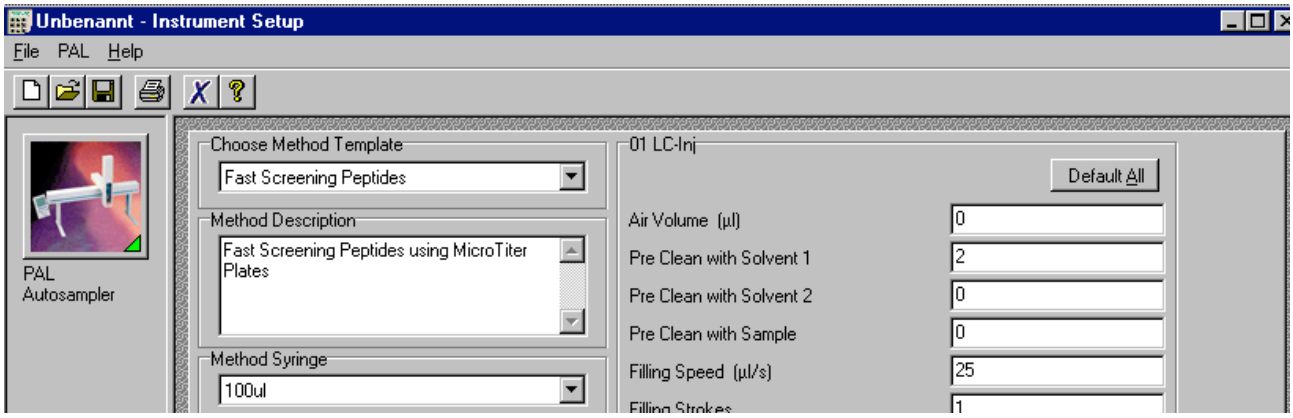
To change or to add a new method Template call the Cycle Composer from the drop-down menu “*PAL*”. This is the actual Method Editor.



Create a new method and use “*save as.*.” to give a unique name.

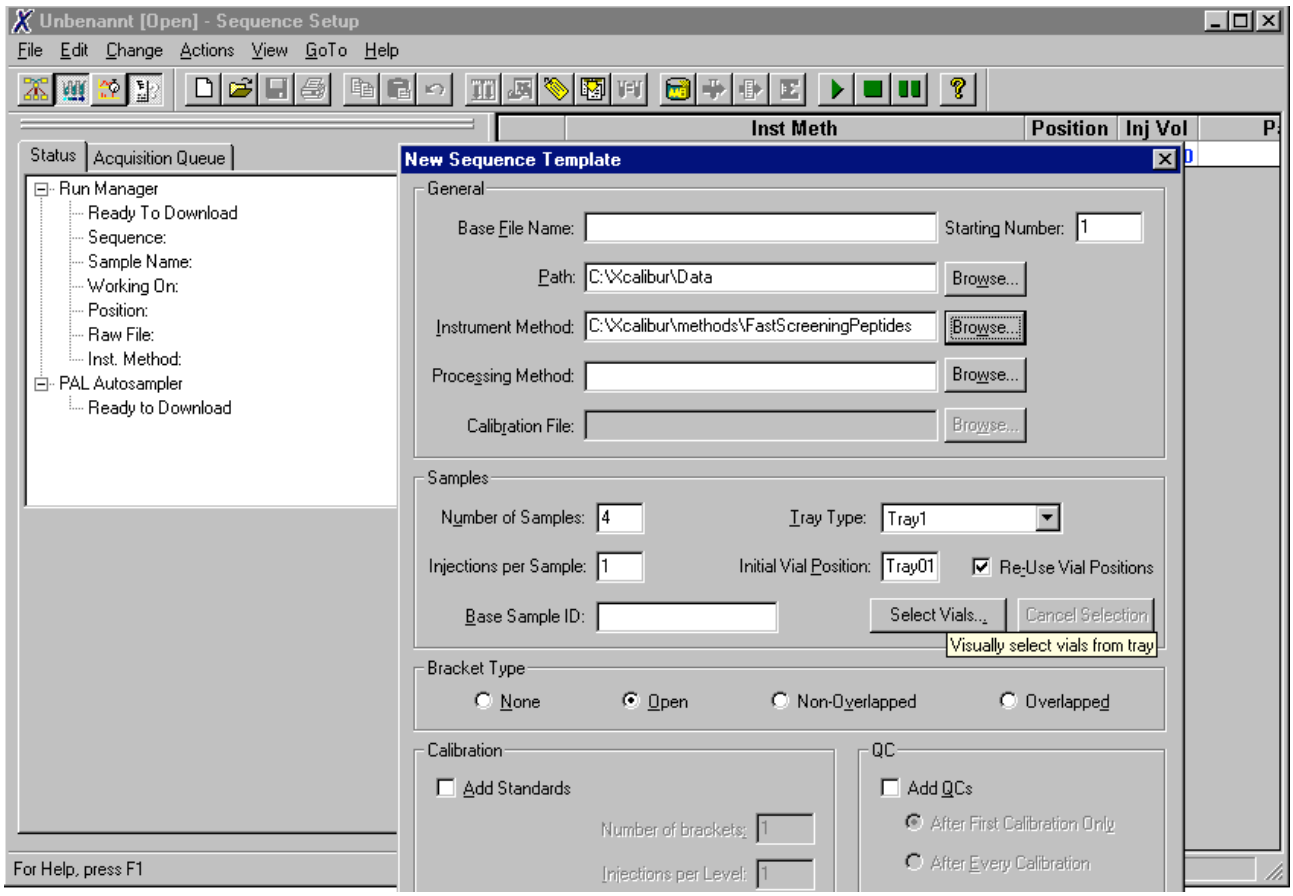


Close the Method Editor and go back to *"Instrument Setup*".
The new created template is now available.



3.3 Sequence Setup

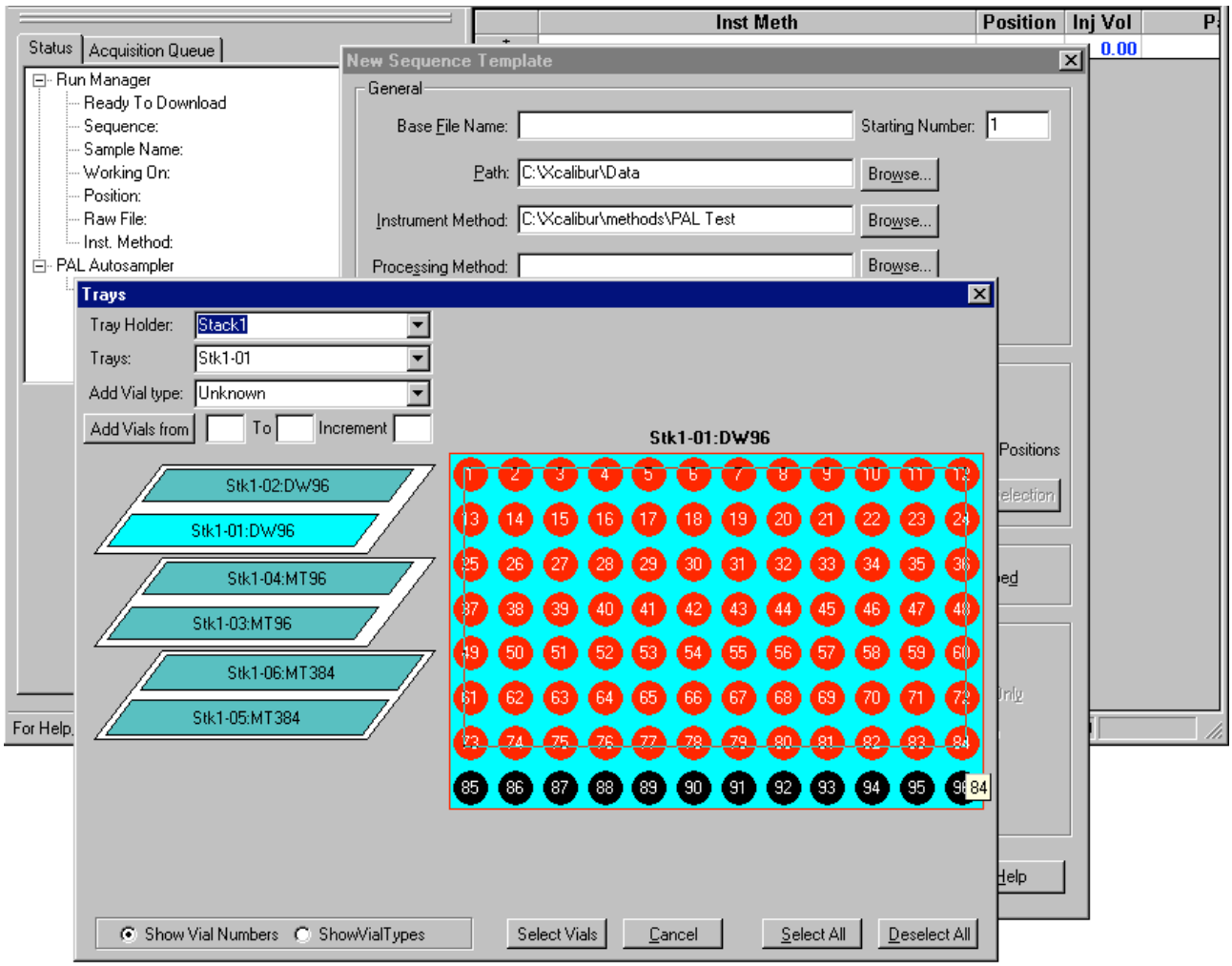
Choose the section "*Sequence Setup*". Select "*New Sequence*" from the menu "*File*".
Fill out the page as described in the Xcalibur manual.



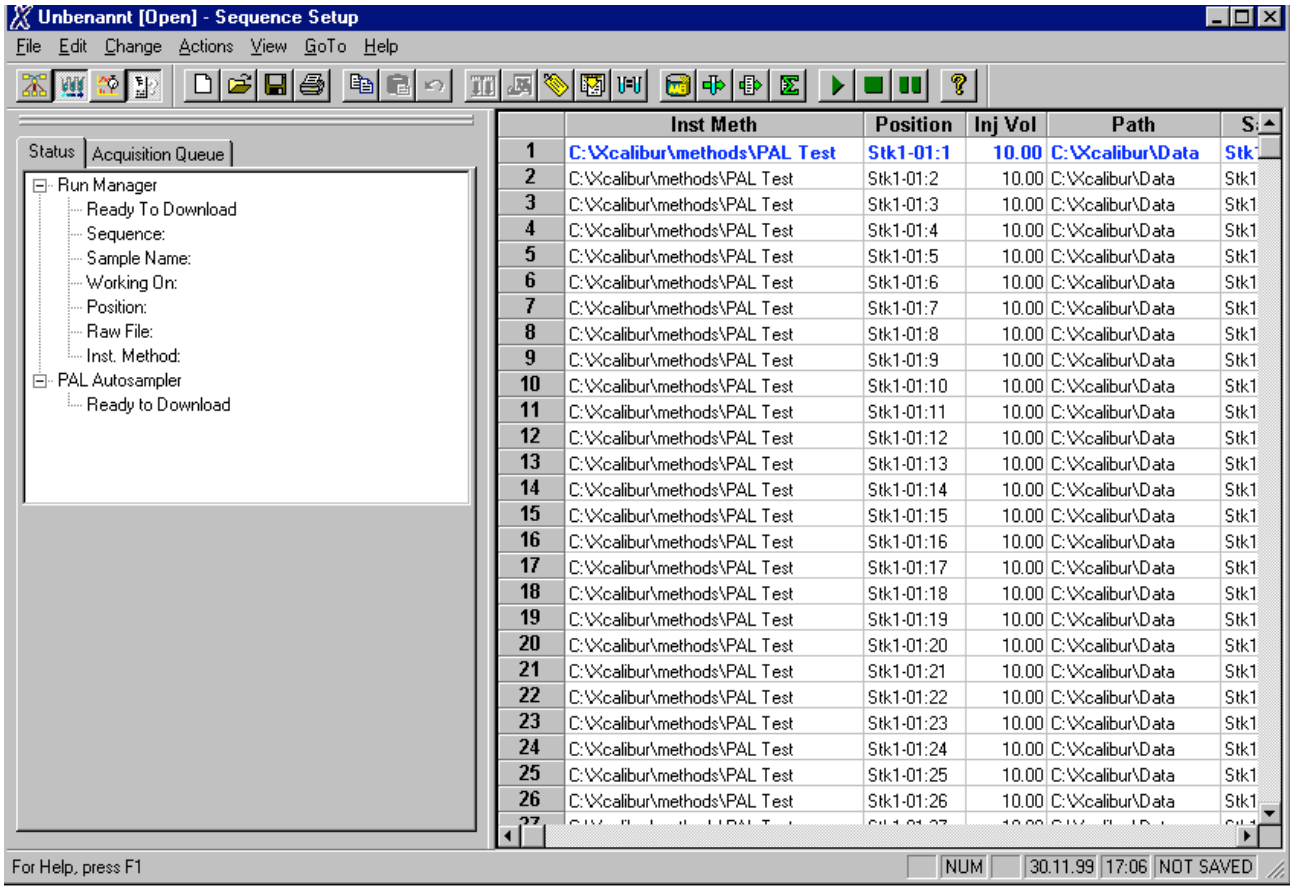
In the section "*Samples*" of the Sequence Template one is confronted with specific buttons for the combination of Xcalibur with the Cycle Composer:

Select *Tray Type*, e. g. Stk1-01
Select Vials

The button "*Select Vial*" will bring the user the full comfort with graphical selection of the vials. CTC highly recommends to use this graphical tool not only for ease-of-use but also to avoid typing errors. The Xcalibur Sequence demands the Tray Name and the Vial Position in one field separated by a colon and the naming of the Tray is case dependent.



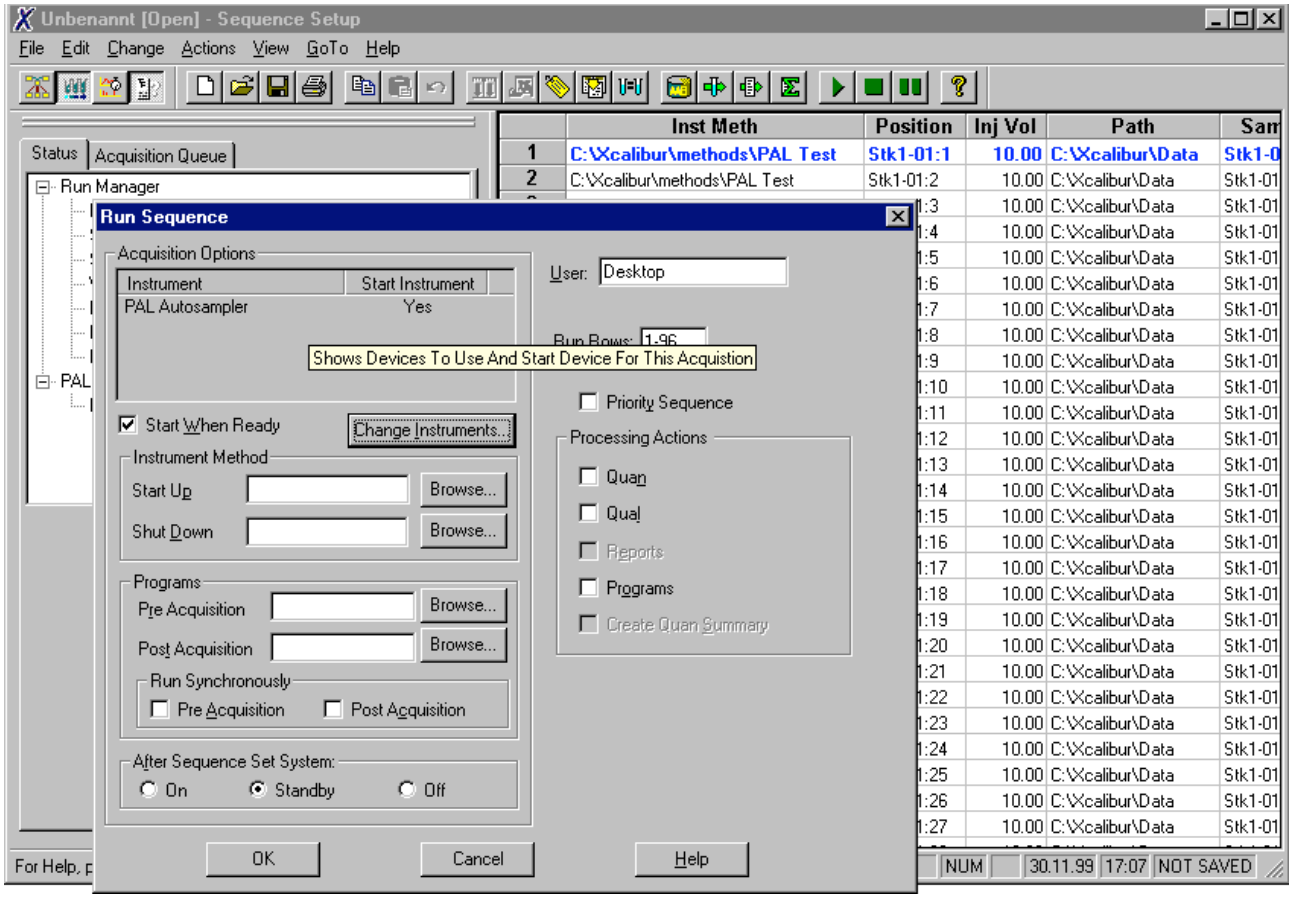
Using the graphical tool from the Cycle Composer will fill out the Sequence List automatically. The Trayholder, Tray and Vial Numbers are entered in the field of "*Positions"* in the Xcalicur specific nomenclature.



3.4 Starting a Sequence

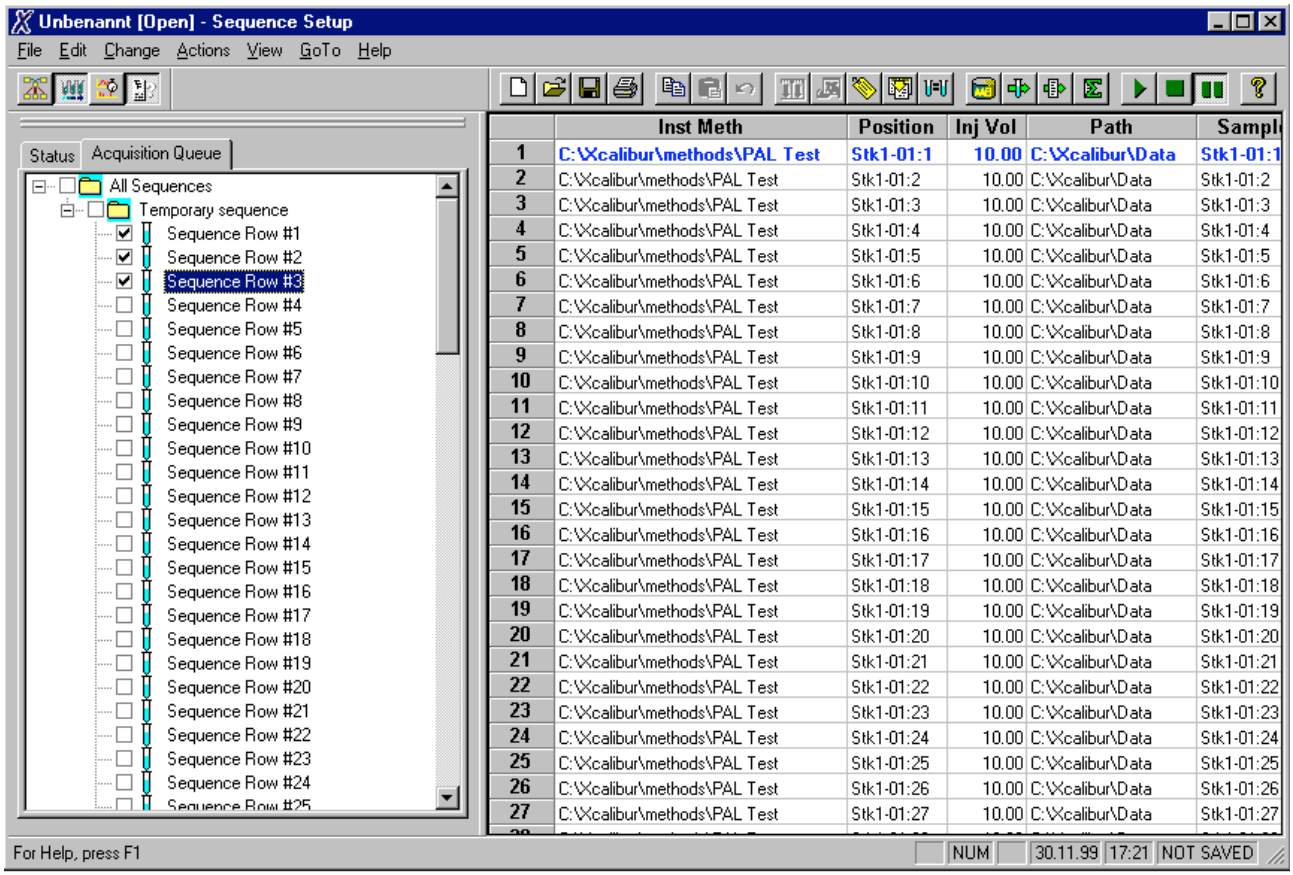
Create with *File/New Sequence* a new Sequence or use the corresponding Icon to start an existing sequence.

A pop-up window "*Run Sequence*" will allow the user to specify the sequence according to his demands.



Specify in the field *"Acquisition Options"* the PAL Autosampler as starting device. Use the button *"Change Instrument"* to enter changes if necessary.

All other parameters for the GC or the HPLC System and the MS-System have to be set and used according to the instruction manuals from the corresponding manufacturer.

The principle of Data Acquisition does not change using the PAL Driver for the Xcalibur Data System. The full comfort of the Xcalibur Software is maintained.

As an example the "*Acquisition Queue*" is displayed.