



# OpenLAB CDS The “Next Generation” of ChemStation and EZChrom Elite



## OpenLAB

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## ADVANCED Session 1

# Maximizing Laboratory Throughput with OpenLAB CDS and Creating Reports with Calculations



Agilent Technologies



# OpenLAB CDS The “Next Generation” of ChemStation and EZChrom Elite

Today’s seminar will demonstrate how to

- Create Custom Fields in ChemStation and EZChrom
- Create and use EZ Sequences
- Queue EZ Sequences for automatic run
- Create single & multi-level Calibration Curves
- Incorporate Custom Fields into OLIR Reports
- Create a variable in OLIR for calculations



# OpenLAB CDS The “Next Generation” of ChemStation and EZChrom Elite

## DEMO

- Create Custom Fields in ChemStation and EZChrom



# Easy Sequence

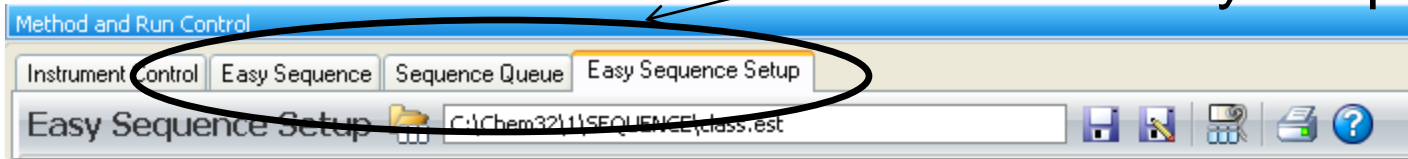
Easy Sequence is a new user interface for quick and easy setup of sequences from templates. In the template, parameters that should be viewed or editable by the user are specified. Calibration setup provides an easy to use drag and drop interface to specify calibration types and sample positions, and displays an overview of the sequence.

**With Easy Sequence, multiple sequences can be submitted to the sequence queue to be run on the data system.**



# Building a Sequence using Easy Sequence

## 3 Tabs for Easy Sequence

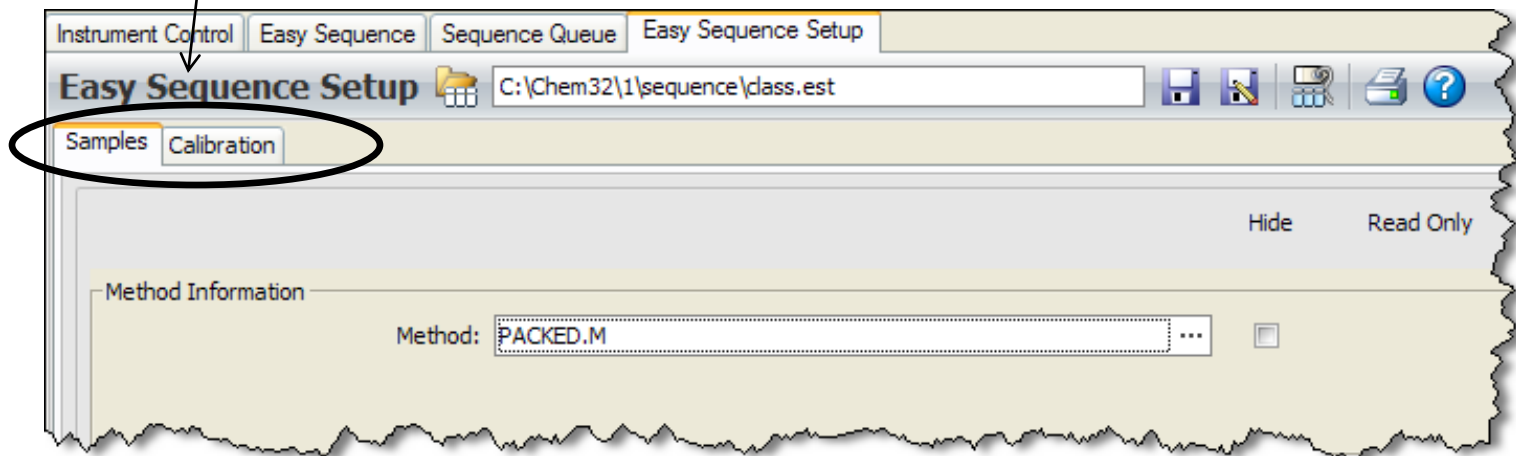


1. Create template using Easy Sequence Setup.
2. Select Sequence Parameters and Sequence Output in **Extended Parameters** screen.
3. Open the template in Easy Sequence and update any required information.
4. Create Easy Sequence by clicking **Fill Samples**.
5. Begin acquisition by clicking **Save and Add to Queue**.



# Easy Sequence Setup

Two panels to set up: Samples and Calibration.







# Easy Sequence Setup - Samples

Instrument Control Easy Sequence Easy Sequence Setup

Easy Sequence Setup C:\Chem32\1\sequence\class.est

Samples Calibration

Hide Read Only

**Injection Location**

Injection Location:  Front  Back

Dual Injection Mode: Custom

**Method Information**

Method: PACKED.M

Back Analysis Method:

**Sample Information**

Starting Vial Location: 104

Number of Samples: 3

Injection Volume: Use Method

Sample Name: sample<C>

Counter Reset (0001) ▶ X

**Data Information**

Data Location: C:\Chem32\1\DATA\

Data File Name: <S><C>

Counter Reset (0001) ▶ X

Sample Name

**Sequence Information**

ence\

Counter Reset (0001) ▶ X

Date and Time

**Easy Sequence Table Columns**

Name	Hide	Read Only	Value
Inj/Vial	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Sample Amount	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0
ISTD Amount	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0
Multiplier	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Dilution	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Lims ID	<input checked="" type="checkbox"/>	<input type="checkbox"/>	
Sample Info	<input type="checkbox"/>	<input type="checkbox"/>	

Specify to create unique filenames.

- Specify which parameters should be hidden or read-only by the user.
- Enter a default value for injections/vial, sample amount, ISTD amount, injection volume, etc.
- Injection, Method, Sample, Data, and Sequence information can also be hidden or read-only.



# Easy Sequence Setup – Extended Parameters

Easy Sequence Setup



- Sequence Parameters

- Sequence Output

A Sequence Summary Report allows you to select from a simple one page Sample Summary to a comprehensive report documenting all aspects of the analysis including cross-sample statistics.

**Extended Parameters: Taft**

Sequence Parameters | Sequence Output

Part of method to run  
According to Runtime Checklist  
According to Runtime Checklist  
Acquisition Only

Wait: 0.00 minutes after loading a new method.

Shutdown  
 Post-Sequence Command/Macro  
macro "SHUTDOWN.MAC".go  
Not Ready Timeout: 0.00 minutes.

**Extended Parameters: Taft**

Sequence Parameters | Sequence Output

Sequence Summary  
 Print sequence summary report Setup...  
 Report to printer  
 Report to file Signal 1: GLPrptF.txt  
Signal 2: GLPrptB.txt  
 Report to PDF  
 Report to HTM  
 Print individual report for each run as well

Individual Reports for each Run  
 As specified in the method  
 As specified here File Settings  
 Printer  .TXT  .EMF  
 Screen  .XLS  .HTM  
 File  .CSV  .DIF  
 .PDF  
 Unique PDF file name  
File prefix: report

OpenLAB Intelligence Reporter  
Browse... Delete

Preview at end of sequence  PDF at end of sequence

OK Cancel Help





# Easy Sequence Setup – GC Dual Injections

- Dual Injection Modes:
  - Custom
  - Throughput
  - Confirmation

Method and Run Control

Instrument Control Easy Sequence Sequence Queue Easy Sequence Setup

Easy Sequence Setup

Samples Calibration

Hide Read Only

Injection Location

Injection Location:  Front  Back

Dual Injection Mode: Custom

Method Information

Method: DUAL.M

Back Analysis Method: DATA ANALYSIS METHOD.M

Sample Information

	Front	Back		
Starting Vial Location:	1	51	<input type="checkbox"/>	<input type="checkbox"/>
Number of Samples:	20	20	<input type="checkbox"/>	<input type="checkbox"/>
Injection Volume:	2	Use Method	<input type="checkbox"/>	<input type="checkbox"/>
Sample Name:			<input type="checkbox"/>	<input type="checkbox"/>

Data Information

Data Location: C:\Chem32\2\DATA\

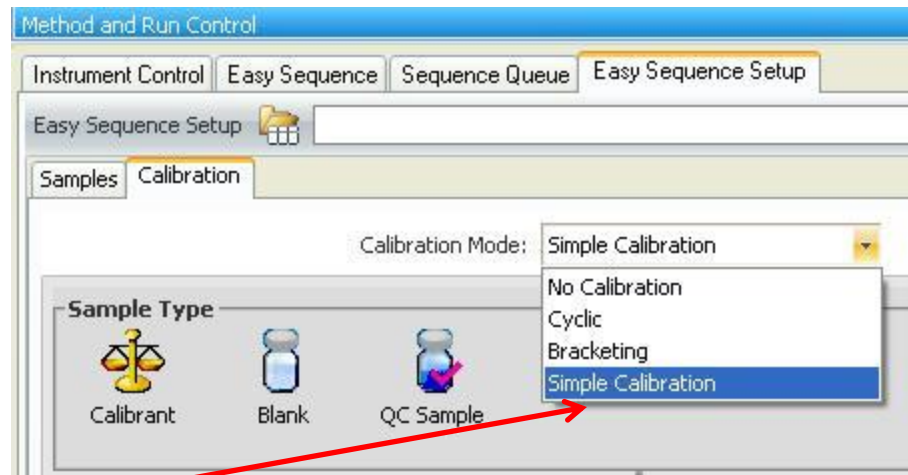
Data File Name:



# Easy Sequence Setup - Calibration

OLCDS C.01.xx: Three choices for Calibration:

- Cyclic
- Bracketing
- Simple Calibration



**Simple Calibration** — Insert a Calibrant, QC Sample, or Blank run at Sequence Start or Sequence End. There are no repeating calibrations.

# Cyclic Recalibration



Instrument Control Easy Sequence Easy Sequence Setup

Easy Sequence Setup C:\Chem32\1\sequence\class.est

Samples Calibration

Calibration Mode: Cyclic

**Sample Type**

Calibrant Blank QC Sample

**Sequence**

Sequence Start

Calibrant

1...n

Cyclic

Calibrant

Calibrant

Calibrant

Injections

Calibration Interval: 3

Interval Unit: Injections

Sequence End

**Calibrant**

Hide Read Only

Calibrant Name: BGC 1C

Vial Location: 103

Injections/Vial: 1

Calibration Level: 3

Update Response Factor: Replace

Update Retention Time: Average

Accept Changes

**Easy Sequence Overview**

Vial 101, BGC 1A, Level (1)

Vial 102, BGC 1B, Level (2)

Vial 103, BGC 1C, Level (3)

3 Injections

Vial 101, BGC 1A, Level (1)

Vial 102, BGC 1B, Level (3)

Vial 103, BGC 1C, Level (3)

3 Injections

3 Injections

Clear All

Drag and drop sample type to appropriate section,

Set parameters.

Preview the recalibration setup.

# Bracketing Recalibration

The screenshot displays the 'Easy Sequence Setup' window with the 'Calibration' tab selected. The 'Calibration Mode' is set to 'Bracketing'. The 'Sample Type' is 'Calibrant'. The 'Sequence' section shows a list of three 'Calibrant' entries under the 'Bracketing' method. The 'Calibrant' configuration panel is active, showing fields for 'Calibrant Name' (BGC 1C), 'Vial Location' (103), 'Injections/Vial' (1), 'Calibration Level' (3), 'Update Response Factor' (Bracket), and 'Update Retention Time' (Average). The 'Easy Sequence Overview' on the right shows a preview of the sequence with three injections for each level.

Instrument Control Easy Sequence Easy Sequence Setup

Easy Sequence Setup C:\Chem32\1\sequence\class.est

Samples Calibration

Calibration Mode: Bracketing

Sample Type  
Calibrant

Drag and drop

Sequence  
1...n  
Bracketing  
Calibrant  
Calibrant  
Calibrant

Calibrant  
Calibrant Name: BGC 1C  
Vial Location: 103  
Injections/Vial: 1  
Calibration Level: 3  
Update Response Factor: Bracket  
Update Retention Time: Average  
Accept Changes

Easy Sequence Overview  
Vial 101 , BGC 1A, Level (1)  
Vial 102 , BGC 1B, Level (2)  
Vial 103 , BGC 1C, Level (3)  
3 Injections  
Vial 101 , BGC 1A, Level (1)  
Vial 102 , BGC 1B, Level (2)  
Vial 103 , BGC 1C, Level (3)  
3 Injections  
Vial 101 , BGC 1A, Level (1)  
Vial 102 , BGC 1B, Level (2)  
Vial 103 , BGC 1C, Level (3)  
Preview the recalibration setup.

Injections  
Calibration Interval: 3  
Interval Unit: Injections

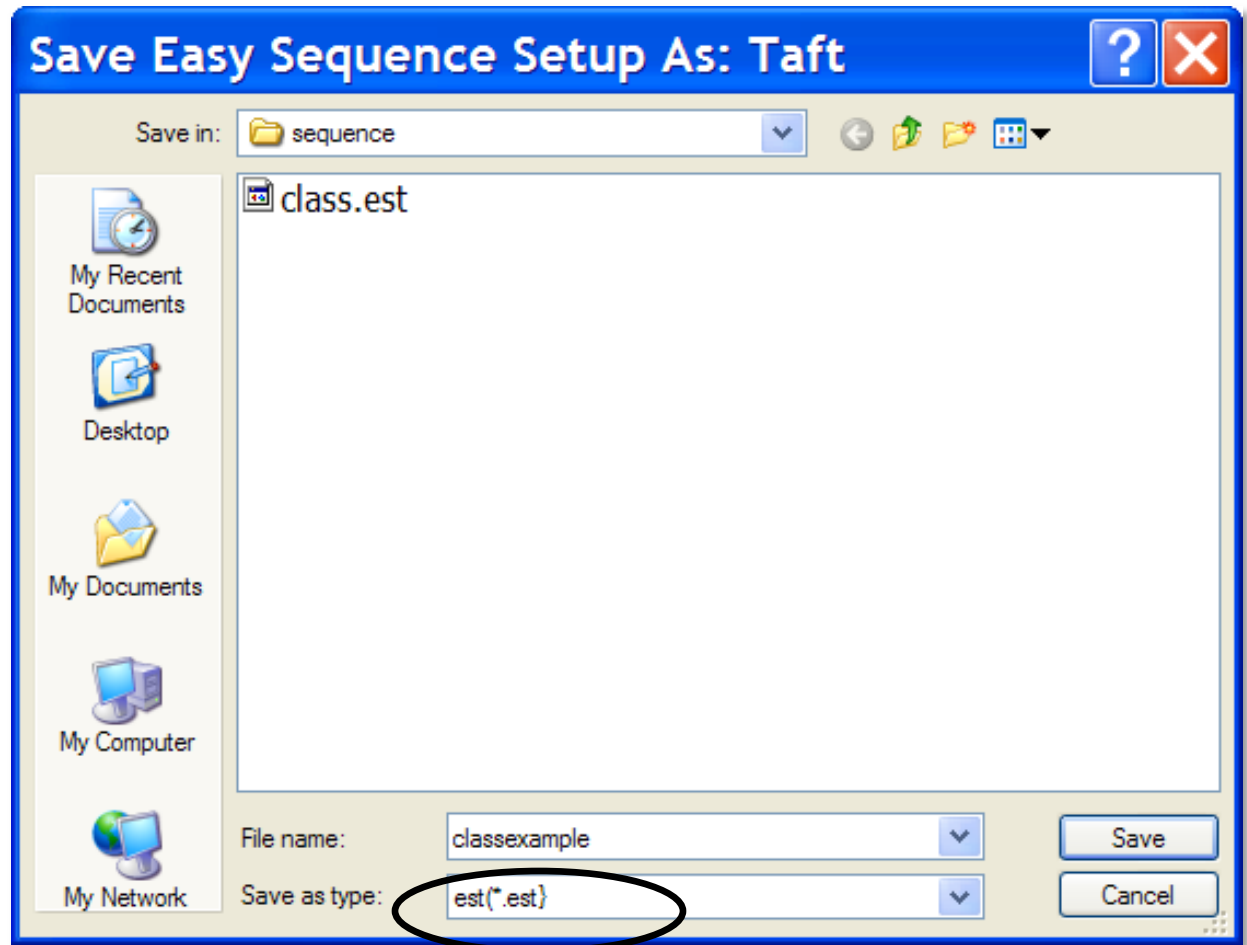
Clear All

Specify for each level

Preview the recalibration setup.



# Save Easy Sequence Setup



# Build Easy Sequence

1. Load the desired Easy Sequence Setup .

Easy Sequence Setup: C:\Chem32\1\sequence\classexample.est

Method Information  
Method: PACKED.M

Data Information  
Data Location: C:\Chem32\1\DATA\  
Data File Name: <S><C>

Sequence Information  
Sequence Location: C:\Chem32\1\sequence\  
Sequence Name: <D>

Sample Information  
Starting Vial Location: 104  
Number of Samples: 3  
Injection Volume: Use Method  
Sample Name: sample<C>

Import Samples... **Fill Samples** Clear Sample List

Vial	Sample Name	Inj/Vial	Inj Volume	Sample Info
> 104	sample0004	1	Use Method	
105	sample0005	1	Use Method	
106	sample0006	1	Use Method	

Preview/Print Sequence... Save and Add to Queue + Automation Engine Version: 1.00 [083] Clear All

2. Fill in number of samples, starting vial, and injections/vial.

3. Select Fill Samples button

4. Preview Sequence

5. Save and Add to Queue.





# Build Easy Sequence

Sample Information

Starting Vial Location:

Number of Samples:

Injection Volume:

Sample Name:

**Sample List** Calibration List

Vial	Sample Name	Inj/Vial	Inj Volume	Sample Info
> 104	sample0001	1	Use Method	
105	sample0002	1	Use Method	
106	sample0003	1	Use Method	

**Sample List** **Calibration List**

Vial	Sample Name	Inj Volume	Sample Info
101	BGC 1A	Use Method	
> 102	BGC 1B	Use Method	
103	BGC 1C	Use Method	
101	BGC 1A	Use Method	
102	BGC 1B	Use Method	
103	BGC 1C	Use Method	

Cyclic Calibration Example  
(cyclic.est)



# Import Samples Sequence


Sample Information

Starting Vial Location:

Number of Samples:

Injection Volume:

Sample Name:

**Import Samples...** 

Fill Samples

Sample List | Calibration List

Vial	Sample Name	Inj/Vial	Inj Volume	Sample Info
104	sample0001	1	Use Method	
105	sample0002	1	Use Method	
106	sample0003	1	Use Method	

Note: Header is required. Exact Text

```
Test3 - Notepad
File Edit Format View Help
SampleLocation, SampleName
104, sample0001
105, sample0002
106, sample0003
```

	A	B
1	SampleLocation	SampleName
2	104	sample001
3	105	sample002
4	106	sample003
5		

Delimited files can be imported.

\*.csv file from Excel

\*.txt file from notepad



# Preview / Print Sequence

Preview/Print Sequence...



## Preview/Print Sequence



Easy Sequence Setup:: cyclic

Method Information

Method: PACKED.M

Data Information

Data Location C:\Chem32\1\DATA\

Data File <S><C>

Sequence Execution

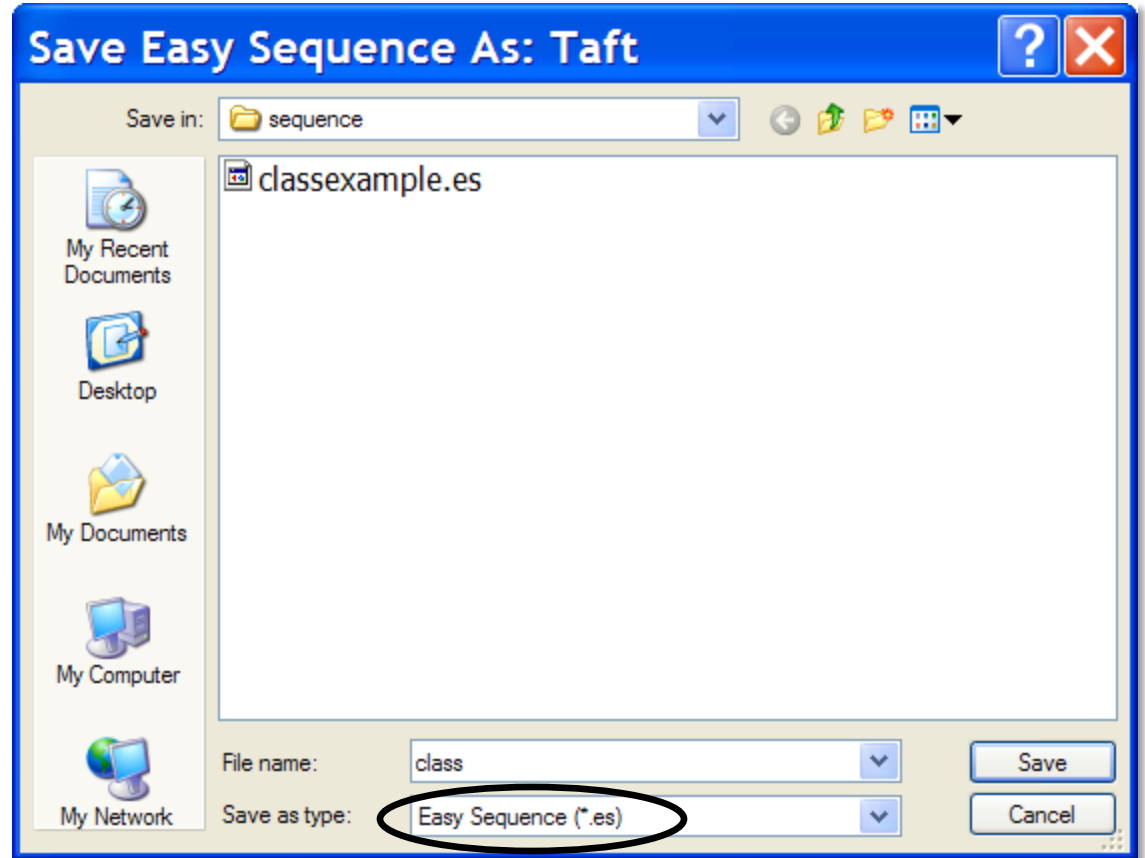
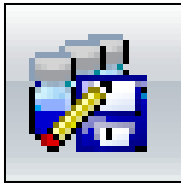
Run	Vial	Sample Name	Inj Volume	Sample Info	Data File	Sample Type	Update RT	Update RF	Cal Level
1	101	BGC 1A	Use Method		BGC 1A0010	Calibrant	Replace	Replace	1
2	102	BGC 1B	Use Method		BGC 1B0011	Calibrant	Replace	Replace	2
3	103	BGC 1C	Use Method		BGC 1C0012	Calibrant	Replace	Replace	3
4	101	BGC 1A	Use Method		BGC 1A0013	Calibrant	Average	Average	1
5	102	BGC 1B	Use Method		BGC 1B0014	Calibrant	Average	Average	2
6	103	BGC 1C	Use Method		BGC 1C0015	Calibrant	Average	Average	3
7	104	sample0010	Use Method		sample00100016	Sample			
8	105	sample0011	Use Method		sample00110017	Sample			
9	106	sample0012	Use Method		sample00120018	Sample			

Print Sequence...

Close



# Save Easy Sequence





# Sequence Queue

Instrument Control Easy Sequence Sequence Queue Easy Sequence Setup

Active Queue: Data System NOT Accepting Sequences (The instrument is not idle.)

Sequences in the Active Queue: 3

Name	Time entered into Queue	Status
class	11/19/2009 2:48 PM	Running
class seq 2	11/19/2009 2:49 PM	Pending
class seq 3	11/19/2009 2:50 PM	Pending

History Queue

Show Sequences that executed in the last 8 hours

Name	Time completed	Status
------	----------------	--------

Pause / Resume Queue

Move Easy Sequence Up

Move Easy Sequence Down

Delete Easy Sequence

Print Active Queue

Edit Sequence... (Pending Status Only)

Hide History Queue

Online Help

Only Pending sequences can be edited (for this instance only)!











# Sequence Queue

- Expand the Sequence in Sequence Queue to show status of each run

Method and Run Control

Instrument Control Easy Sequence **Sequence Queue** Easy Sequence Setup

Active Queue: Data System Accepting Sequences

Sequences in the Active Queue: 1        


Name	Time entered into Queue	Estimated Completion Time	Status
pcb2	4/21/2010 10:54:18 AM		Pending

Run Number	Location	Name	Method	Start Time	Status
1	1 (Front)/51 (Back)	(Front)/(Back)	DUAL.M		Pending
2	2 (Front)/52 (Back)	(Front)/(Back)	DUAL.M		Pending
3	3 (Front)/53 (Back)	(Front)/(Back)	DUAL.M		Pending

History Queue

Show Sequences that executed in the last 8 hours 

Name	Time completed	Status
pcb1	4/21/2010 4:52:34 AM	Aborted
sequence 2	4/21/2010 4:50:06 AM	Stopped
sequence 1	4/21/2010 3:35:38 AM	Error





# Sequence Queue Considerations

Multiple sequences can be added to the queue.

The Easy Sequence acquisition begins as soon as the data system is ready.

Once an Easy Sequence is started, it cannot be changed from the Sequence Queue. It becomes a ChemStation sequence (.s) and the Sequence Table must be edited.

Only pending easy sequences in the queue can be edited from the Sequence Queue.