

SFC User's Booklet

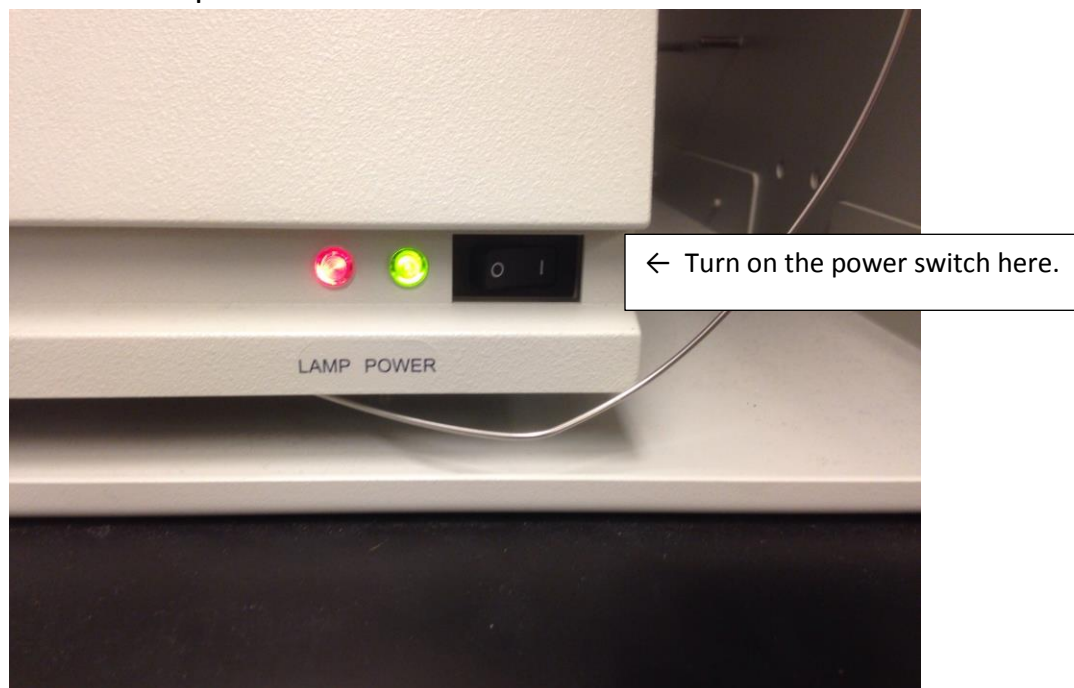
Please note:

You cannot use any of these solvents:

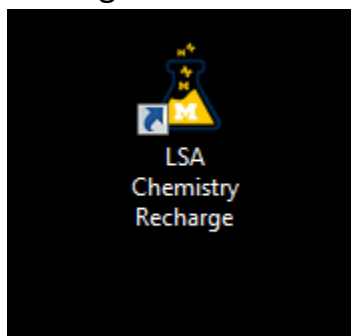
Acetone, Chloroform, Methylene Chloride, DMF, DMSO, Ethyl Acetate, THF. Even small amounts of these solvents will destroy the expensive chiral columns!

Acceptable solvents are methanol, isopropanol, and acetonitrile.

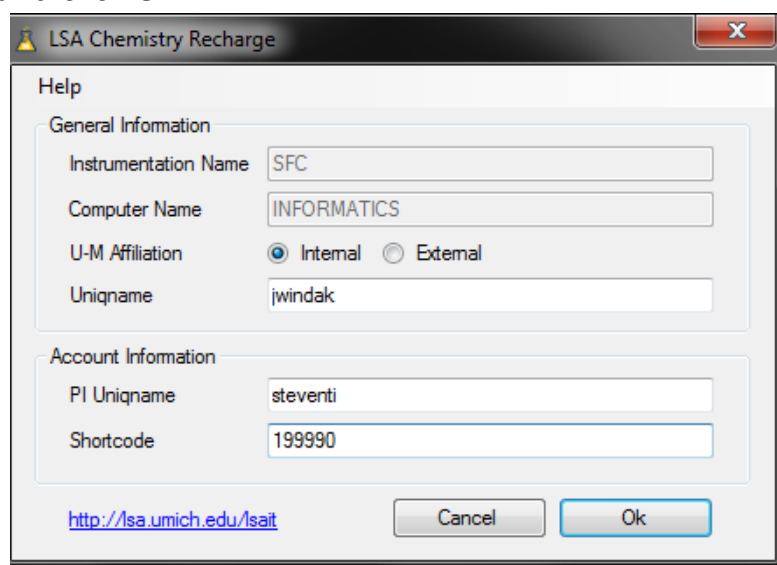
- 1) Turn on the power switch for the UV-Detector:



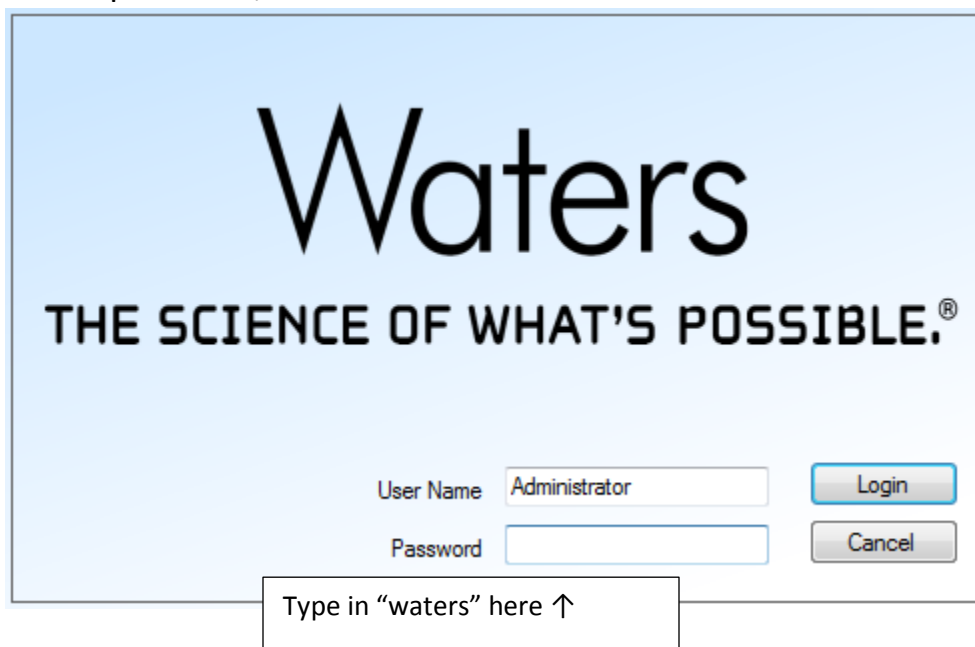
2) Double-Click the LSA Chemistry Recharge Icon:



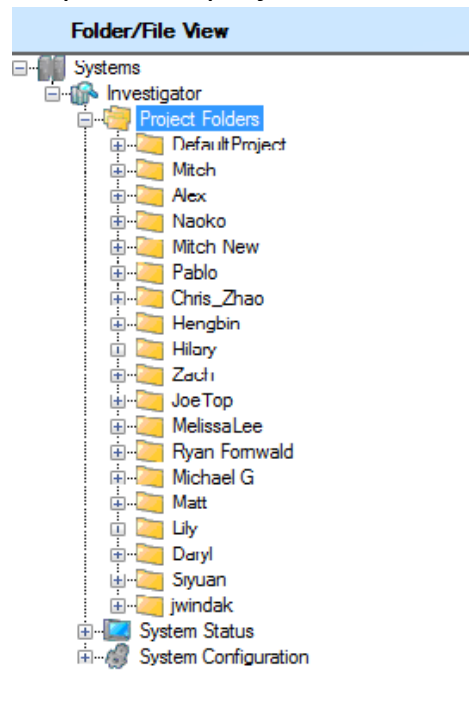
3) Fill in your uniqueness, your research advisor's uniqueness, and your shortcode account number, and click OK.

A dialog box titled 'LSA Chemistry Recharge' with a 'Help' icon and a close button. It contains two sections: 'General Information' and 'Account Information'.
General Information:
Instrumentation Name: SFC
Computer Name: INFORMATICS
U-M Affiliation: Internal External
Uniqname: jwindak
Account Information:
PI Uniqname: steventi
Shortcode: 199990
At the bottom, there is a URL <http://lsa.umich.edu/lsait> and 'Cancel' and 'Ok' buttons.

The Waters Chromscope software will open automatically.
When it asks for a password, enter "waters"

The Waters logo is displayed in large black font, with the tagline 'THE SCIENCE OF WHAT'S POSSIBLE.®' below it. At the bottom, there are fields for 'User Name' (containing 'Administrator') and 'Password' (empty). To the right of the 'User Name' field is a 'Login' button, and to the right of the 'Password' field is a 'Cancel' button. A callout box points to the password field with the text 'Type in "waters" here ↑'.

4) After the software comes up, expand the project folders to find your project:



5) Expand your project and instrument methods to see your methods. Choose a method to run.

The screenshot shows a 'Folder/File View' window with a tree structure. The tree is expanded to show 'Instrument Methods' under 'Method Files'. A callout box with an arrow points to 'Instrument Methods' with the text '← click on Instrument methods'. Below the tree, a 'Name' field shows 'Jim.cmf' with another callout box pointing to it with the text '← choose a method to run and click on it'.

Folder/File View

- Systems
 - Investigator
 - Project Folders
 - Default Project
 - Mitch
 - Alex
 - Naoko
 - Mitch New
 - Pablo
 - Chris_Zhao
 - Hengbin
 - Hilary
 - Zach
 - Joe Top
 - Melissa Lee
 - Ryan Formwald
 - Michael G
 - Matt
 - Lily
 - Daryl
 - Styuan
 - jwindak
 - Sequence Files
 - Method Files
 - Instrument Methods**
 - Integration Methods
 - Collection Methods
 - Data Files
 - Report Templates
 - History Folders
 - Jim2
 - System Status
 - System Configuration

← click on Instrument methods

Name

Jim.cmf

← choose a method to run and click on it

6) Your method will be displayed. If all is correct, you can click on Run Method.

For a Chiral column scan, it is suggested to use a flow rate of 3.5 ml/min, a co-solvent percentage of 10% to 20%, and a back-pressure of 120 Bar, and a temperature of 40 C.

Please note, the chiral columns should not be heated above 40 C.

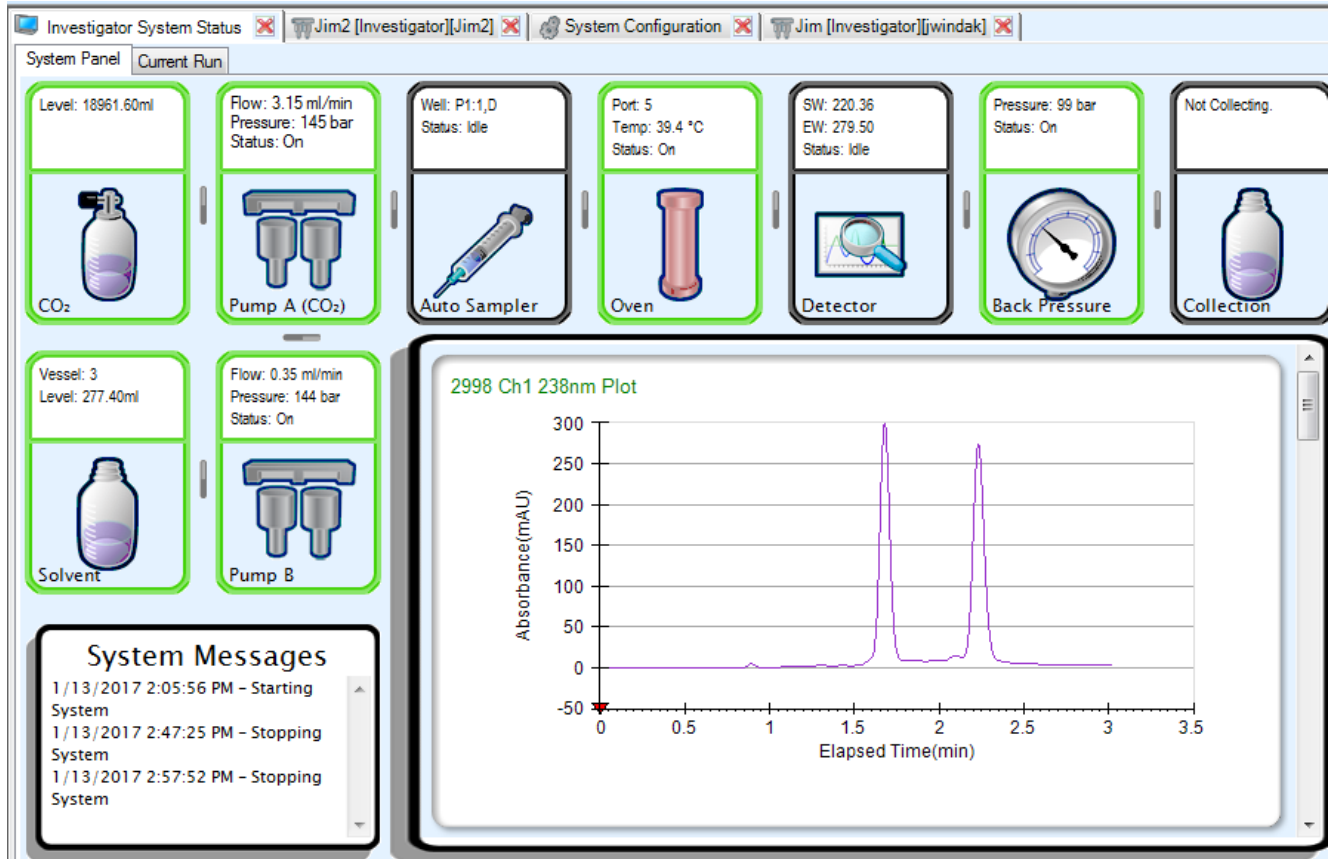
The screenshot displays the 'General Method' configuration window in the Investigator software. The 'Method Name' is 'Jim'. The 'Flow' section is set to 'Isocratic' with a 'Total Flow (ml/min)' of 3.50. The 'Temperature (C)' is 40. The 'Default Column*' is '5: AD-H Chiral An' and the 'Default Solvent*' is '3: iPrOH'. The 'Composition' section is set to 'Isocratic' with a 'Co-Solvent %' of 10.00. The 'Pressure' section is set to 'Isobaric' with a 'Total Back Pressure (bar)' of 120. A note states: '*Note: Default Columns and Solvents can be overridden in the sequence.'

Below the configuration fields is a table with columns: Stage, Total Start Flow (ml/min), Total End Flow (ml/min), Duration (min), and a Delete button. The table contains two rows:

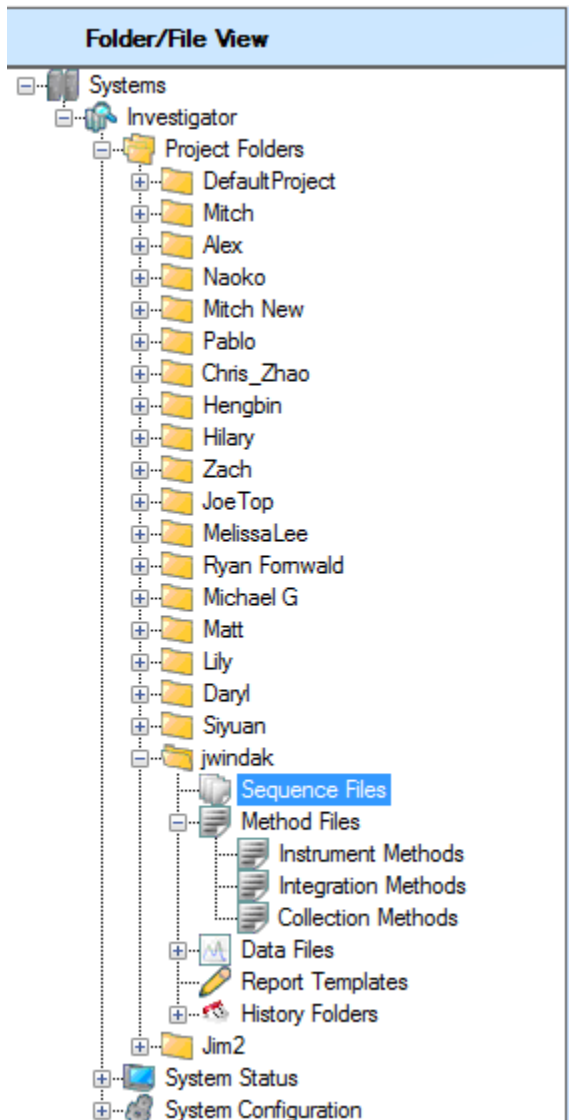
Stage	Total Start Flow (ml/min)	Total End Flow (ml/min)	Duration (min)	Delete
1	3	0	1	Delete
2				

At the bottom, there is a 'Graph Display' section with radio buttons for 'Flow', 'Composition', and 'Pressure'. The 'Flow' radio button is selected. The graph is titled 'Flow Gradient Display' and shows a linear decrease in flow rate from 3 ml/min at 0 minutes to 0 ml/min at 1 minute. The x-axis is 'Total Gradient Duration (min)' ranging from 0 to 1.5, and the y-axis is 'Flow Rate (ml/min)' ranging from 0 to 3.

- 7) Click on “Investigator System Status” to obtain status information on the system. If a module has a yellow colored boarder, it means it is not ready. If it has a green colored boarder, it is ready and is operating properly. If a module has a black colored boarder, it is ready but not currently being in use.



8) Right-click on Sequence Files, and then left-click “Add New Sequence To”



You can then fill out the sequence table for your list of sample runs:

Sequence Queue: [Icons]

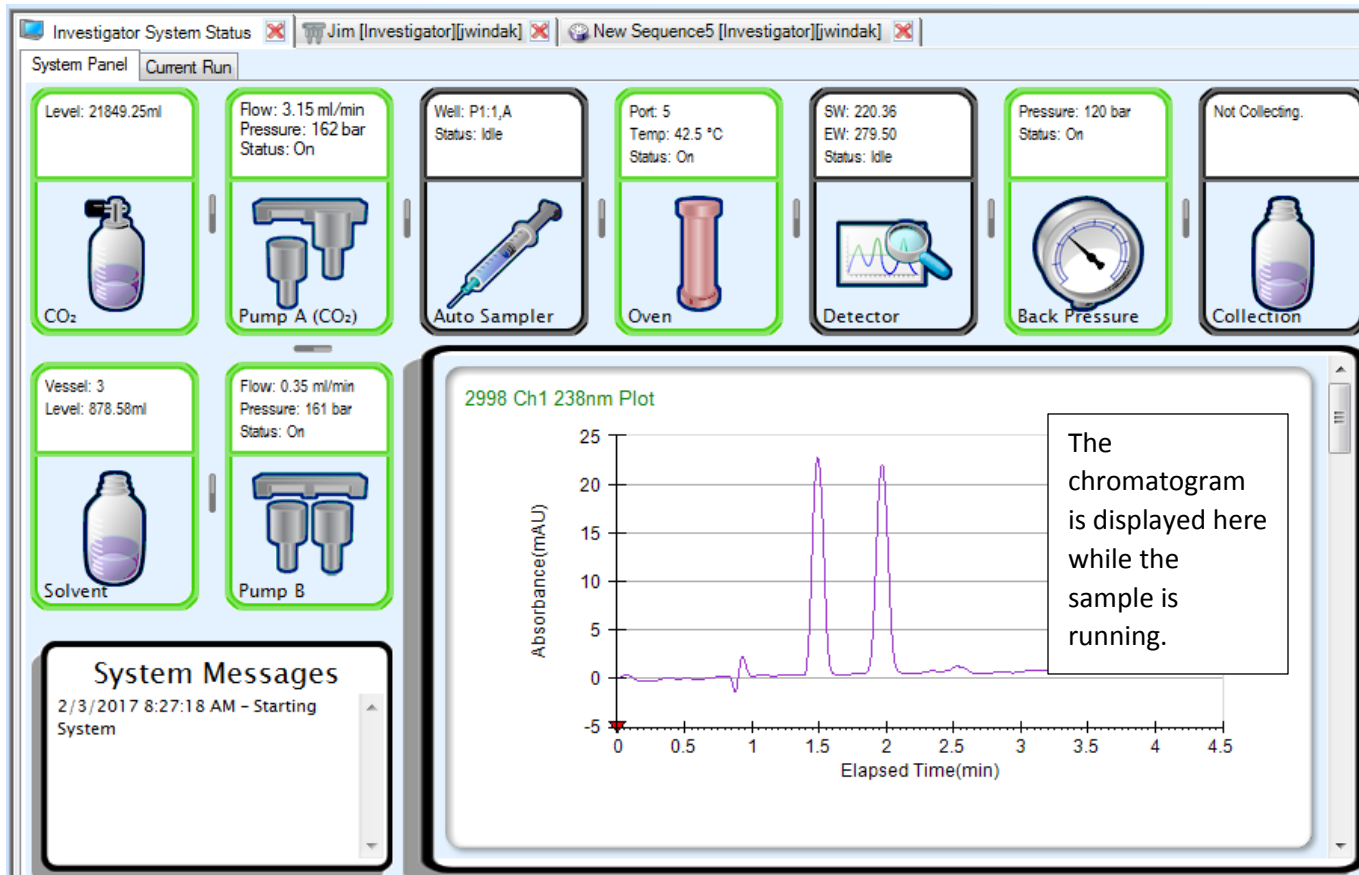
Current Project: [Field]
 Current Method(s): IM: Jim[Ver: 190]
 Current Data File: [Field]
 Run: [Field] of [Field]
 In Sequence: [Field]

Lamp Auto-off Time: 0.48 of 30.00 min.

Sequence Name: New Sequence5 Version 0 [Save] [Add to Queue] [Sequence Wizard]
 Created By: [Field] Total Duration (min) 11.1
 Make a single acquisition for entire sequence

Inj. #	Run. Dur. (min.)	Inj. Delay (min.)	Instrument Method	Data File	Inj. Loc.	Sample Name	Inj. Vol. (uL)	Solvent	Column	Collection Method
1	10	0	Jim	Sample Name And Date/Time	1,1,A	racemic mixture 1]	10	Use Method Def...	Use Method Def...	
*										

After the sequence table is filled out, click on Save and then Add to Queue. Click on Start to begin running the sequence.



How to do a Chiral Method Screening:

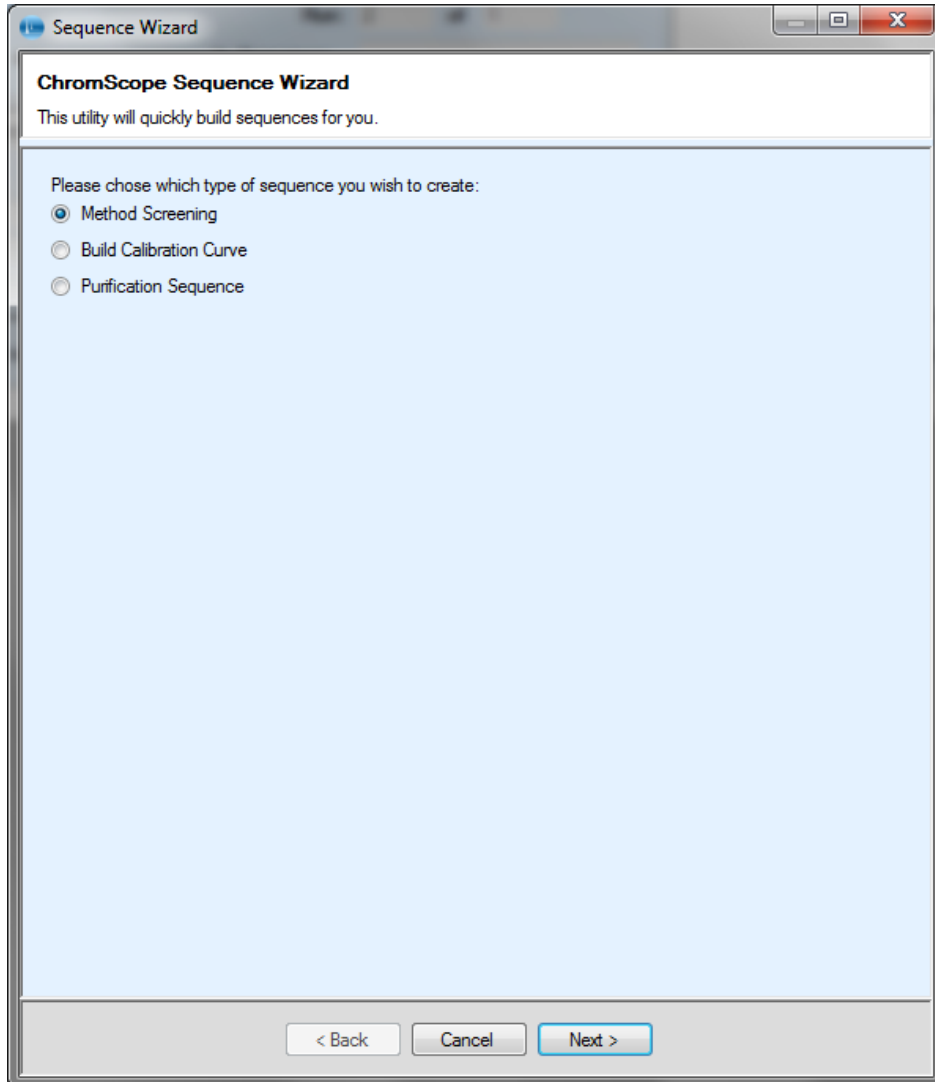
- 1) Right-click "sequence files", and then click on "Add new sequence to", and the sequence table will be displayed. After it is displayed, click on the button that says "Sequence Wizard":

The screenshot shows the 'New Sequence' dialog box. The 'Sequence Name' is 'New Sequence6', 'Version' is '0', and 'Total Duration (min)' is '0'. There are buttons for 'Save', 'Add to Queue', and 'Sequence Wizard'. A checkbox labeled 'Make a single acquisition for entire sequence' is present. Below the dialog is a table with the following columns:

Inj. # *	Run. Dur. (min.)	Inj. Delay (min.)	Instrument Method *	Data File *	Inj. Loc. *	Sample Name *	Inj. (C)
*							

A callout box with a downward arrow points to the 'Sequence Wizard' button, with the text: "Click on Sequence Wizard ↓".

It will ask you what type of sequence you want to create. Click on “Method Screening” and then click on Next:



A Dialog box will come up, allowing you to choose what needs to be changed from run to run. In this example, we've used the same solvent but have chosen to cycle through all of the chiral columns:

ChromScope Sequence Wizard
This utility will quickly build sequences for you.

Method Screening Settings:

Samples to screen: * 1,1.A
Change First

Solvents to screen: *
Change Third

- MeOH
- Solvent 2
- iPrOH
- Solvent 4
- AcN
- 0.2% TEA in iPrOH

Instrument methods to screen: *
Change Second

- Jim

Columns to screen: *
Change Last

- Silica Analytical
- BEH-2EP Semi-Prep
- AS-H Chiral Analytical
- OJ-H Chiral Analytical
- AD-H Chiral Analytical
- OD-H Chiral Analytical
- IA Chiral Analytical
- IB Chiral Analytical
- IC Chiral Analytical
- ID Chiral Analytical

Run duration: * 3.00 min.

Injection volume: * 10.00 uL

Equil time on change: 1.00 min.

of injections per sample: * 1

Equil time between every inj.: 0.00 min.

Data file: * Sample Name And Date/Time

Integration method:

Report template:

Report Template Print Options:

User notes:

< Back Cancel OK

Click on OK, and the sequence table will automatically be set up for all of the runs:

Sequence Name: New Sequence6 Version: 0
Created By: Total Duration (min): 40.8

Make a single acquisition for entire sequence

Inj. #	Run. Dur. (min.)	Inj. Delay (min.)	Instrument Method	Data File	Inj. Loc.	Sample Name	Inj. Vol. (uL)	Solvent	Column
1	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	AS-H Chiral Ana...
2	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	OJ-H Chiral Ana...
3	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	AD-H Chiral An...
4	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	OD-H Chiral An...
5	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	IA Chiral Analyti...
6	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	IB Chiral Analyti...
7	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	IC Chiral Analyti...
8	3	1	Jim	Sample Name And Date/Time	1,1.A	sbd-III-198	10	iPrOH	ID Chiral Analyti...

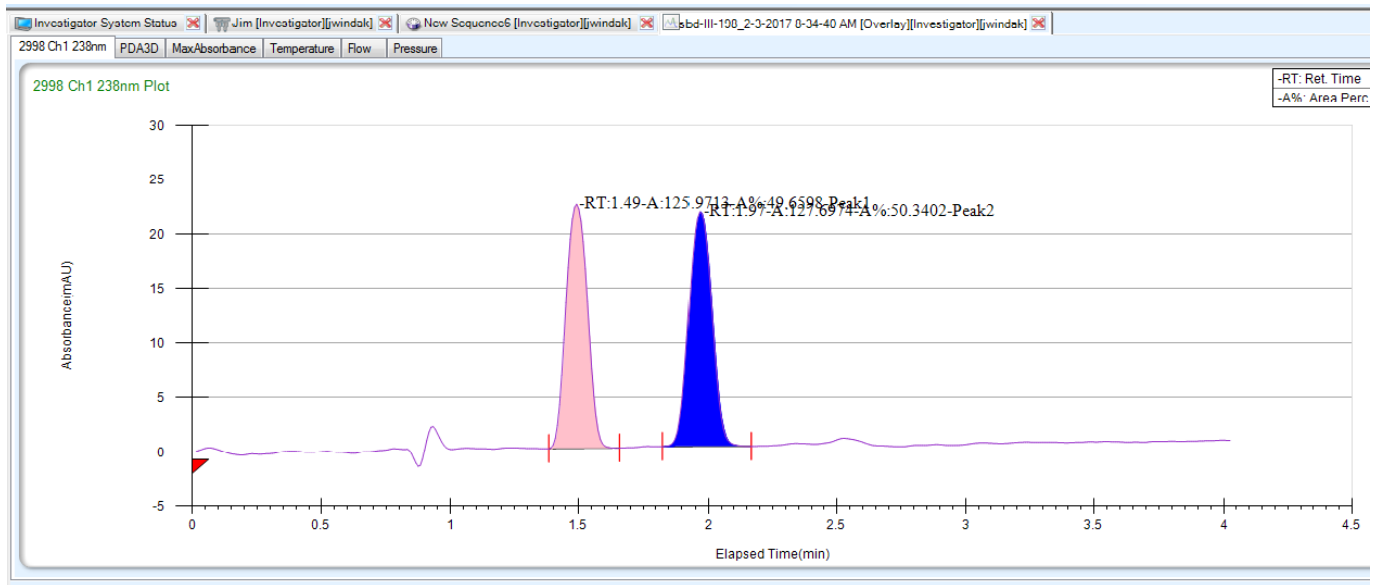
Click on Save, and then click on Add to Queue, and then start the run.

How to Display Data Files That Have Been Run:

The screenshot shows a software interface with a file tree on the left and a list of files on the right. The file tree is expanded to show the 'Data Files' folder, which contains a 'Monitor' sub-folder. The 'Monitor' sub-folder is expanded to show a list of dates from 11_16_2016 to 2_3_2017. The date '2_3_2017' is selected. A callout box points to the 'Data Files' folder with the text '← Expand your Data files folder'. Another callout box points to the '2_3_2017' folder with the text '← Click on the folder with the date you want to display'. A third callout box points to the list of files with the text '← The list of data files will be displayed here. Double-click the one you want to view'. The list of files is as follows:

Name
sbd-III-198_2-3-2017 8-28-40 AM.tta
sbd-III-198_2-3-2017 8-34-40 AM.tta
sbd-III-198_2-3-2017 8-57-42 AM.tta
sbd-III-198_2-3-2017 9-02-37 AM.tta
sbd-III-198_2-3-2017 9-07-30 AM.tta
sbd-III-198_2-3-2017 9-13-13 AM.tta
sbd-III-198_2-3-2017 9-18-29 AM.tta
sbd-III-198_2-3-2017 9-23-22 AM.tta
sbd-III-198_2-3-2017 9-28-14 AM.tta
sbd-III-198_2-3-2017 9-33-08 AM.tta

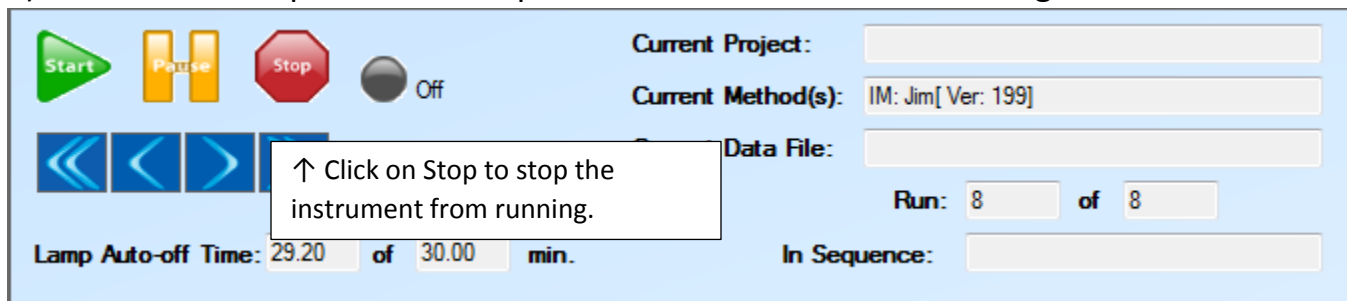
Your data file will then be displayed:



To print a report, or save one as a PDF, click on the File menu, and click on "Print Quick Report to Printer" or "Print Quick Report to PDF".

How to Shut Down the System When Done:

1) Click on the Stop button to stop the current method from running:



2) Close the Chromscope software. Closing the software will close your billing account.

3) Turn off the power switch for the UV Detector:

