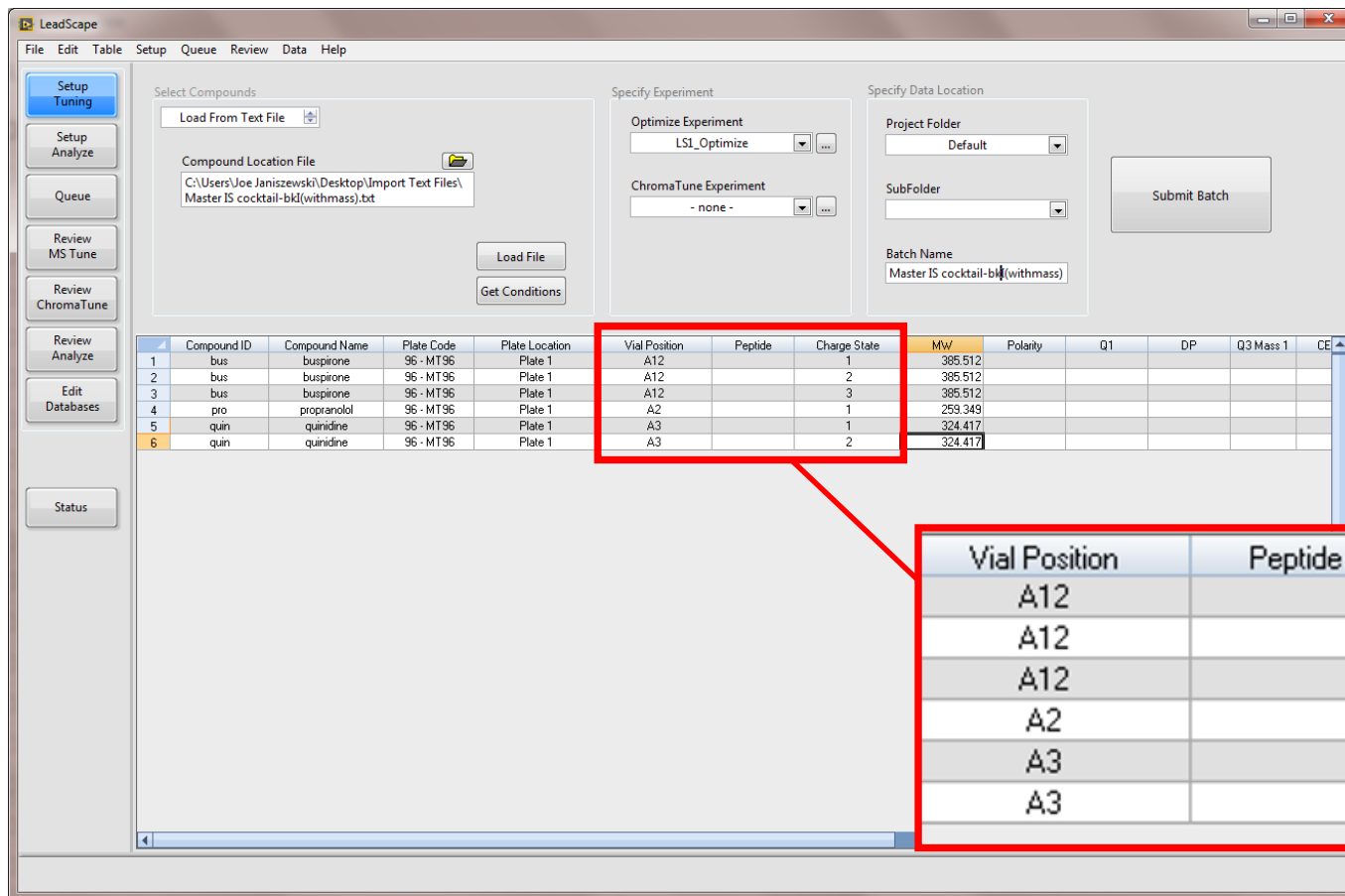


LeadScape Workflow Peptide Optimization

- Setup: Inject from the same well for multiple charge states
- Review: Wells with multiple injections are marked with ‘
- Review each charge state using well pull down, wells with multiple injections are labelled: well #-injection#
- Use keyboard arrow keys to switch between each charge state result

Setup of Optimize for Charge States

- Inject sample multiple times from the same well
- Set charge state for each optimization



LeadScope

File Edit Table Setup Queue Review Data Help

Setup Tuning

Setup Analyze

Queue

Review MS Tune

Review ChromaTune

Review Analyze

Edit Databases

Status

Select Compounds

Load From Text File

Compound Location File

C:\Users\Joe Janiszewski\Desktop\Import Text Files\Master IS cocktail-bk(withmass).txt

Load File

Get Conditions

Specify Experiment

Optimize Experiment

LSI_Optimize

ChromaTune Experiment

- none -

Specify Data Location

Project Folder

Default

SubFolder

Batch Name

Master IS cocktail-bk(withmass)

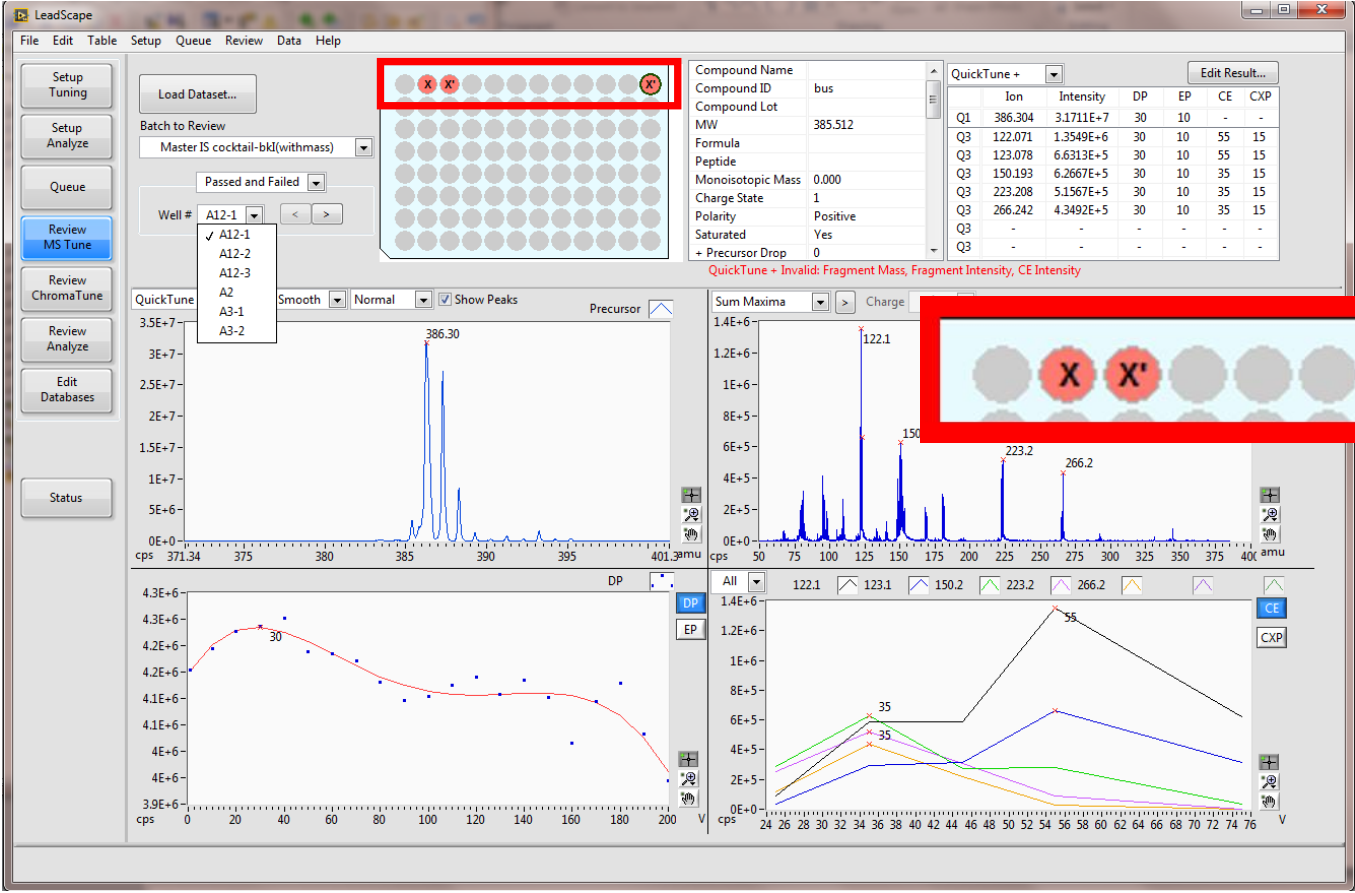
Submit Batch

Compound ID	Compound Name	Plate Code	Plate Location	Vial Position	Peptide	Charge State	MW	Polarity	Q1	DP	Q3 Mass 1	CE
1	bus	busprone	96 - MT96	Plate 1	A12	1	385.512					
2	bus	busprone	96 - MT96	Plate 1	A12	2	385.512					
3	bus	busprone	96 - MT96	Plate 1	A12	3	385.512					
4	pro	propranolol	96 - MT96	Plate 1	A2	1	259.349					
5	quin	quinidine	96 - MT96	Plate 1	A3	1	324.417					
6	quin	quinidine	96 - MT96	Plate 1	A3	2	324.417					

Vial Position	Peptide	Charge State
A12		1
A12		2
A12		3
A2		1
A3		1
A3		2

Review of Multi Injected Wells

- Wells sampled multiple times denoted with ' in plate diagram
- Well # menu lists injection number for wells injected multiple times



The screenshot shows the LeadScope software interface. At the top, a plate diagram highlights several wells with 'X' and 'X'' markers. A dropdown menu for 'Well #' is open, showing options A12-1, A12-2, A12-3, A2, A3-1, and A3-2. The main display area contains two mass spectra: a 'Sum Maxima' plot and a 'Charge' plot. The 'Sum Maxima' plot shows peaks at 122.1, 150.2, 223.2, and 266.2. The 'Charge' plot shows peaks at 35 and 55. A table of ion data is visible in the top right corner.

Ion	Intensity	DP	EP	CE	CXP
Q1	386.304	3.1711E+7	30	10	-
Q3	122.071	1.3549E+6	30	10	55
Q3	123.078	6.6313E+5	30	10	55
Q3	150.193	6.2667E+5	30	10	35
Q3	223.208	5.1567E+5	30	10	35
Q3	266.242	4.3492E+5	30	10	35
Q3	-	-	-	-	-
Q3	-	-	-	-	-

Proposed Peptide Workflow

- Setup Tuning: Optimize Compound at each charge state
- Review MS Tune: Review Optimization results
- Setup Tuning: Based on Optimization batch, perform ChromaTune on each charge state
- Review ChromaTune: Review ChromaTune response
- Review ChromaTune: Select Best tunes based on Opt and CT results
- Review ChromaTune: Selected Tunes are marked via the Tune Comment, e.g. [multiCS frag=1,3]
- Setup Analyze: Retrieve best tune in Analyze Setup based on presence of [multiCS....] in comment field in Optimization Record

Optimize for each charge state

- Inject from the same well, choose a different charge state for each injection
- Make injections of the compound sequential to allow easy review of each injection

The screenshot shows the LeadScape software interface. The main window is titled "LeadScape" and has a menu bar with "File", "Edit", "Table", "Setup", "Queue", "Review", "Data", and "Help". On the left side, there is a vertical toolbar with buttons for "Setup Tuning", "Setup Analyze", "Queue", "Review MS Tune", "Review ChromaTune", "Review Analyze", "Edit Databases", and "Status". The main area is divided into three sections: "Select Compounds", "Specify Experiment", and "Specify Data Location".

Select Compounds: A "Load From Text File" button is at the top. Below it, the "Compound Location File" field contains the path "C:\Users\Joe Janiszewski\Desktop\Import Text Files\Master IS cocktail-bk(withmass).txt". There are "Load File" and "Get Conditions" buttons.

Specify Experiment: The "Optimize Experiment" dropdown is set to "LS1_Optimize". The "ChromaTune Experiment" dropdown is set to "- none -".

Specify Data Location: The "Project Folder" dropdown is set to "Default". The "SubFolder" dropdown is empty. The "Batch Name" field contains "Master IS cocktail-bk(withmass)". A "Submit Batch" button is located to the right.

At the bottom, there is a table with the following data:

	Compound ID	Compound Name	Plate Code	Plate Location	Vial Position	Peptide	Charge State	MW	Polarity	Q1	DP	Q3 Mass 1	CE
1	bus	buspirone	96 - MT96	Plate 1	A12		1	385.512					
2	bus	buspirone	96 - MT96	Plate 1	A12		2	385.512					
3	bus	buspirone	96 - MT96	Plate 1	A12		3	385.512					
4	pro	propranolol	96 - MT96	Plate 1	A2		1	259.349					
5	quin	quinidine	96 - MT96	Plate 1	A3		1	324.417					
6	quin	quinidine	96 - MT96	Plate 1	A3		2	324.417					

CT for each charge state

- CT will optimize each charge state, if run independently of the MS Tune
- If the CT tune is linked to the MS Tune only the most recent data will be used, which will be for a single charge state.

- Optimized for 2 Charge States
- Run 2 CT injections with same formatting as Optimization

The screenshot shows the LeadScope software interface. On the left, there is a vertical toolbar with buttons for 'Setup Tuning', 'Setup Analyze', 'Queue', 'Review MS Tune', 'Review ChromaTune', 'Review Analyze', 'Edit Databases', and 'Status'. The main window is divided into several sections: 'Select Compounds' (with a dropdown menu showing 'CS05', 'multiCS-04', 'ChargeState03', 'multiCS-02', and 'multiCS-01'), 'Specify Experiment' (with 'Optimize Experiment' set to '- none -' and 'ChromaTune Experiment' set to 'multiCS'), and 'Specify Data Location' (with 'Project Folder' set to 'Default'). A 'Submit Batch' button is located on the right. At the bottom, a table displays data for two compounds. The table has columns for Compound ID, Vial Position, MW, Monoisotopic Mass, Formula, Peptide, Q1, and seven Q3 Mass values (Q3 Mass 1 through Q3 Mass 7). Red arrows point from the text on the left to the 'Review Analyze' button and the table.

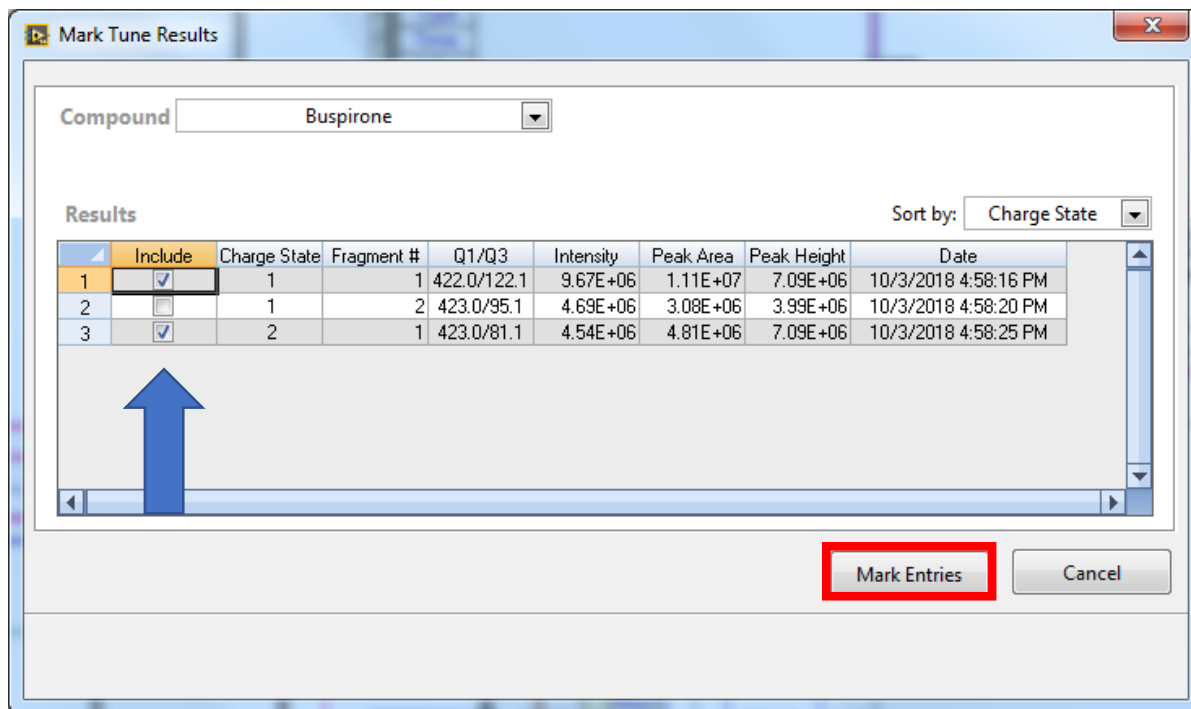
Compound ID	Vial Position	MW	Monoisotopic Mass	Formula	Peptide	Q1	Q3 Mass 1	Q3 Mass 2	Q3 Mass 3	Q3 Mass 4	Q3 Mass 5	Q3 Mass 6	Q3 Mass 7
1	8	1099.573	1099.573	TDRPSQQLR	TDRPSQQLR	551.082	436.309	403.346	175.213	212.198	159.179	183.243	493.864
2	8	1099.573	1099.573	TDRPSQQLR	TDRPSQQLR	560.160	550.342	436.309	871.644	660.532	774.602	589.474	403.346

Review CT Results

- TBD

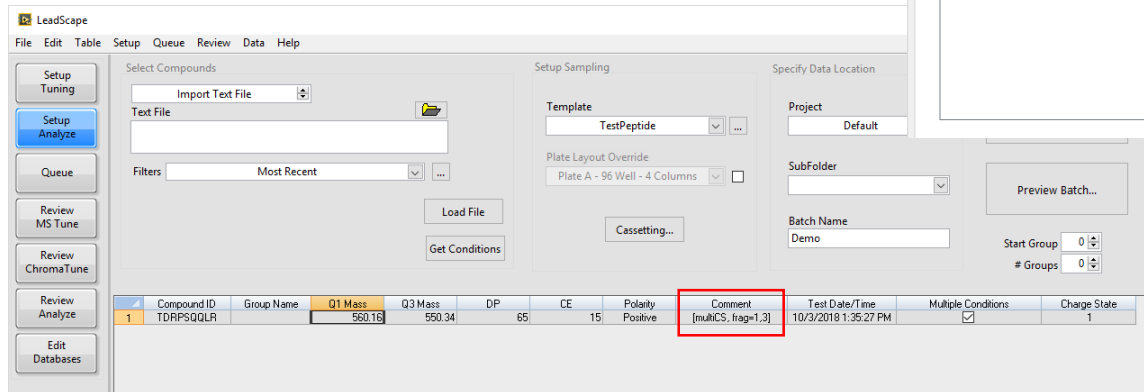
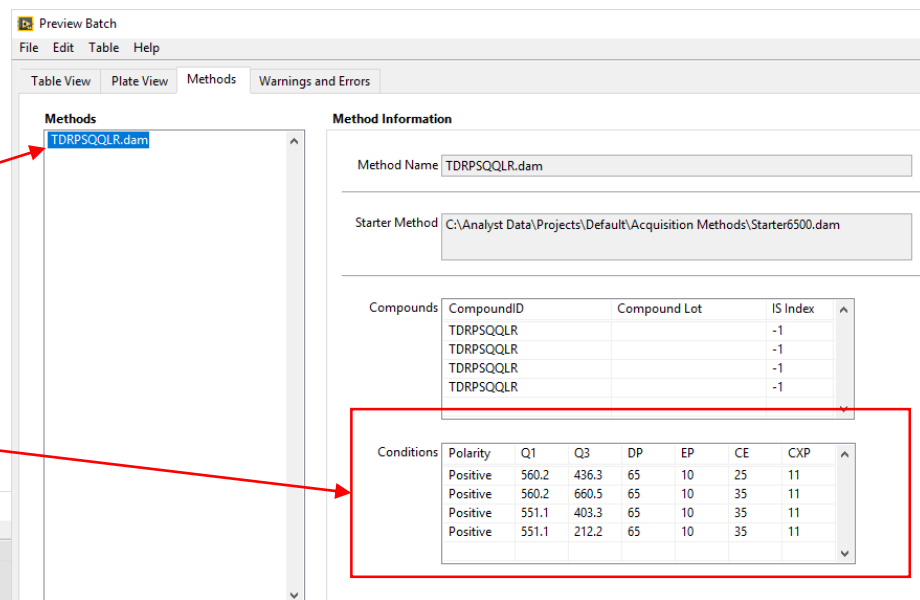
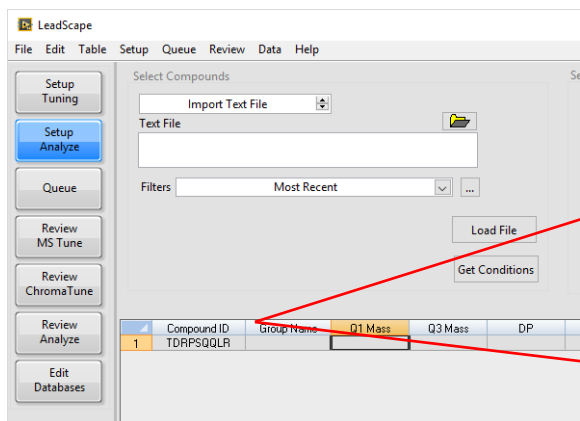
Mark Selected Tune

- Select Compound from the list
- Results table will be populated with the MS Tune and CT injection results
- Can sort by any of the table fields to help with selection
- Check Tunes to mark in the database
- Repeat for next compound
- When all compound have been evaluated press Mark Entries to commit the changes to the database.



Retrieve Selected Tune

- Analyze Setup will retrieve the tune based on the marked entries.
- If marked tunes exist Analyze Setup will create batches using the marked Charge State/Fragment entries.
- If no marked tunes exist the method building will work as in the current version of LeadScope.



- Version 1.0 – 3 October 2018
- Created by Wayne Lootsma