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LeadScape Workflow
Peptide Optimization

Current Workflow

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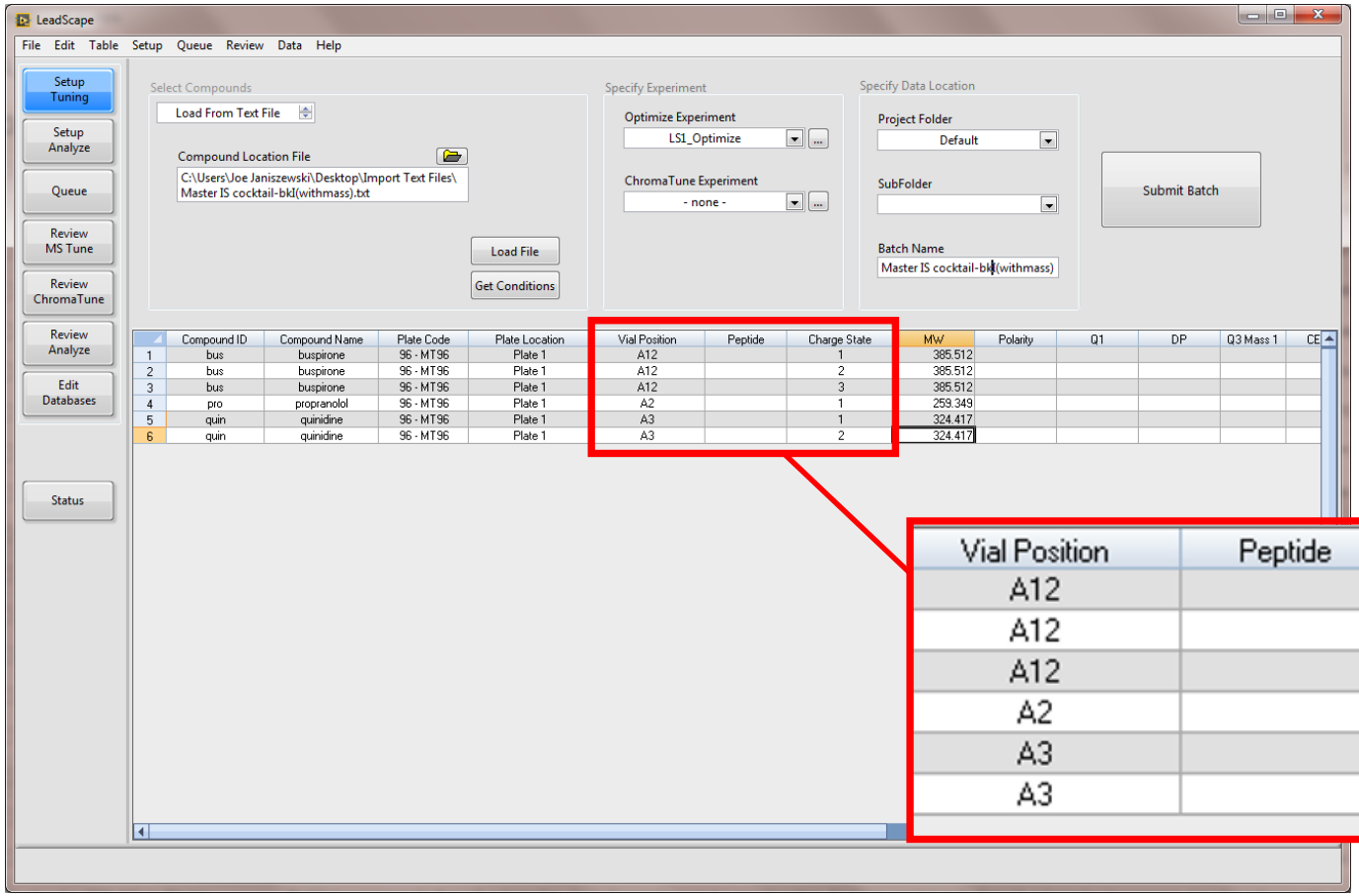
- Setup: Inject from the same well for multiple charge states
- Review: Wells with multiple injections are marked with ‘
- Review each charge state using well pull down, wells with multiple injections are labelled: well #-injection#
- Use keyboard arrow keys to switch between each charge state result

Setup of Optimize for Charge States

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



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

Review of Multi Injected Wells

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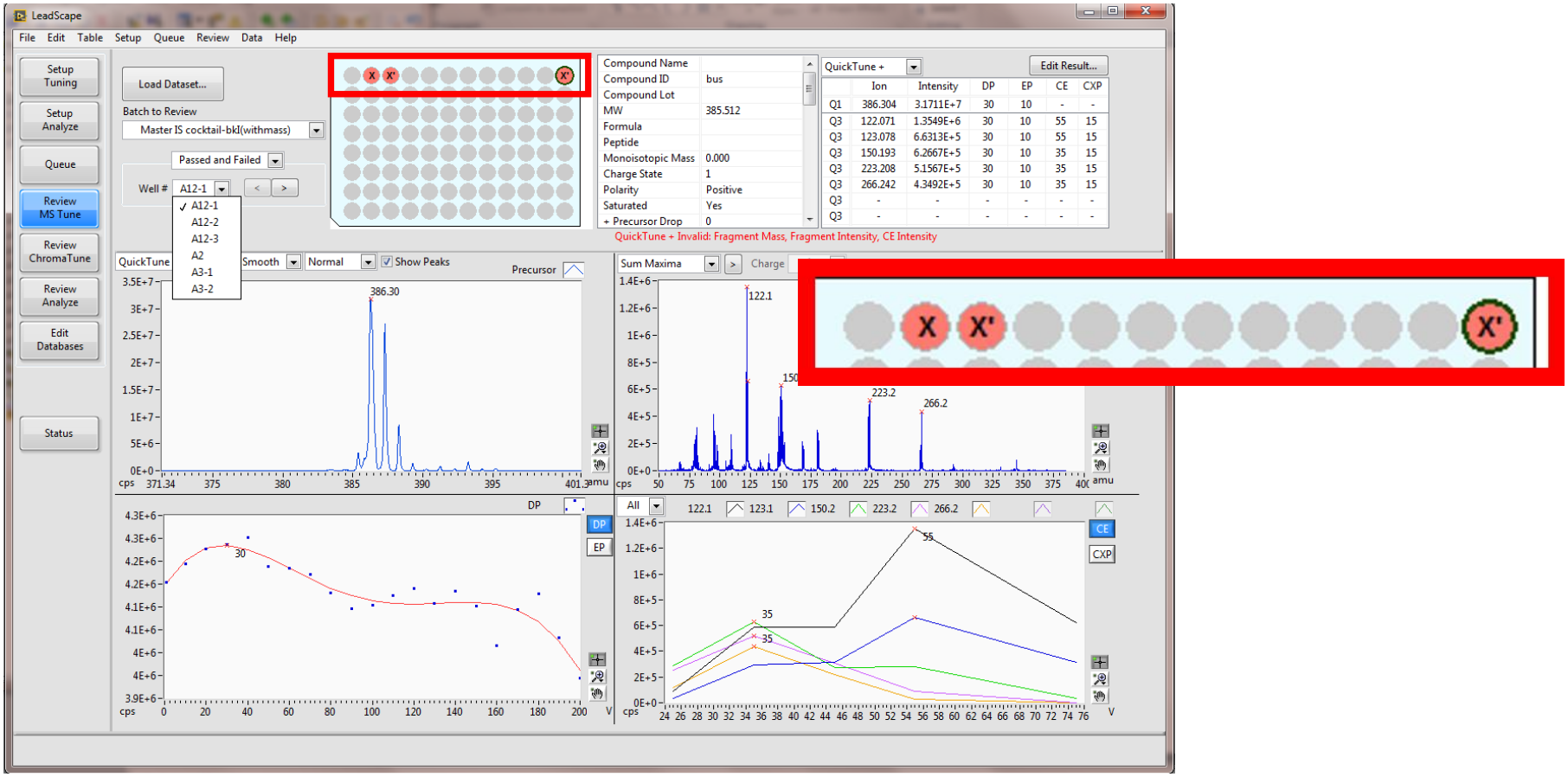
- Wells sampled multiple times denoted with ‘ in plate diagram
- Well # menu lists injection number for wells injected multiple times



Proposed Peptide Workflow

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- 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

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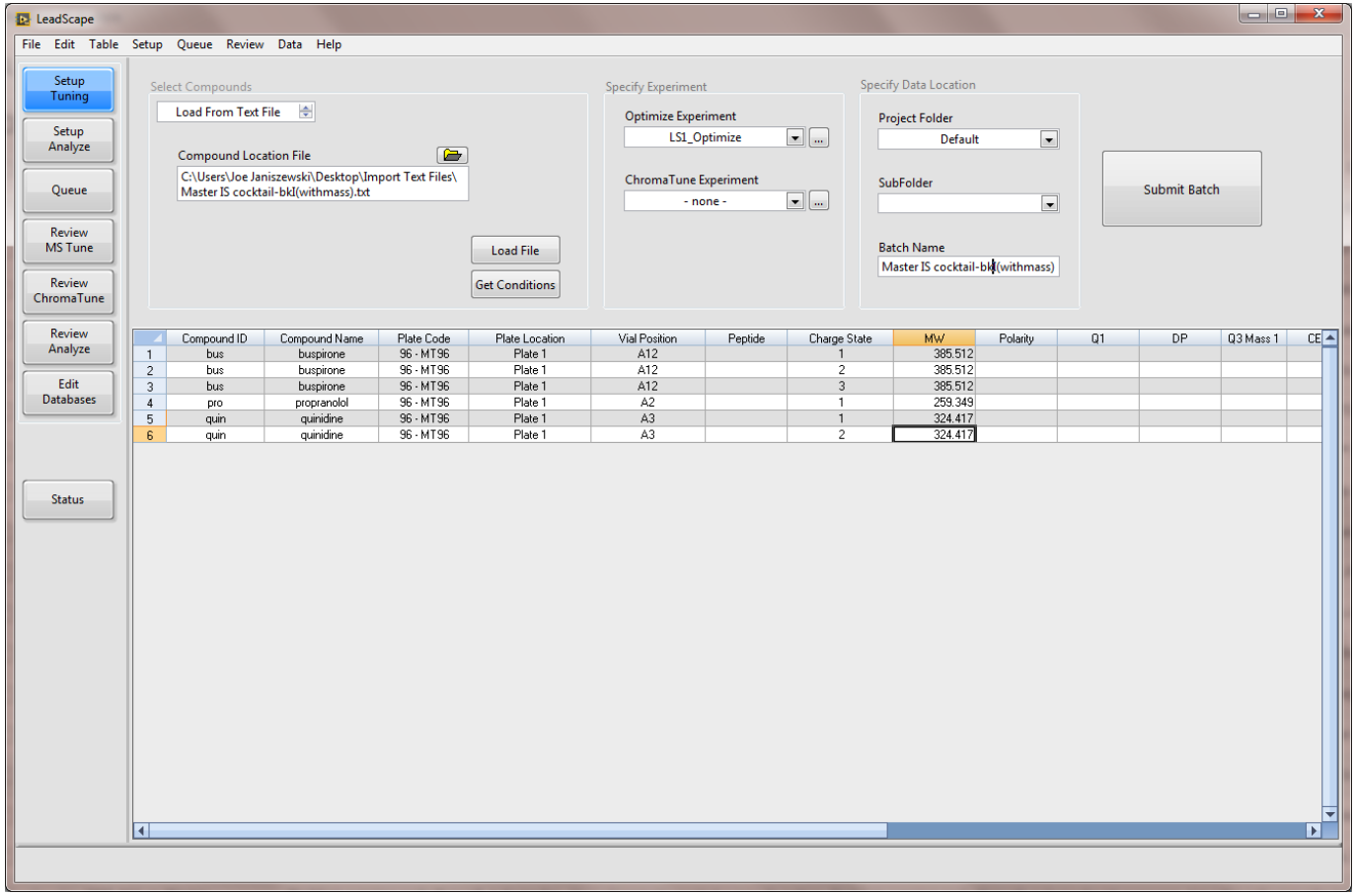
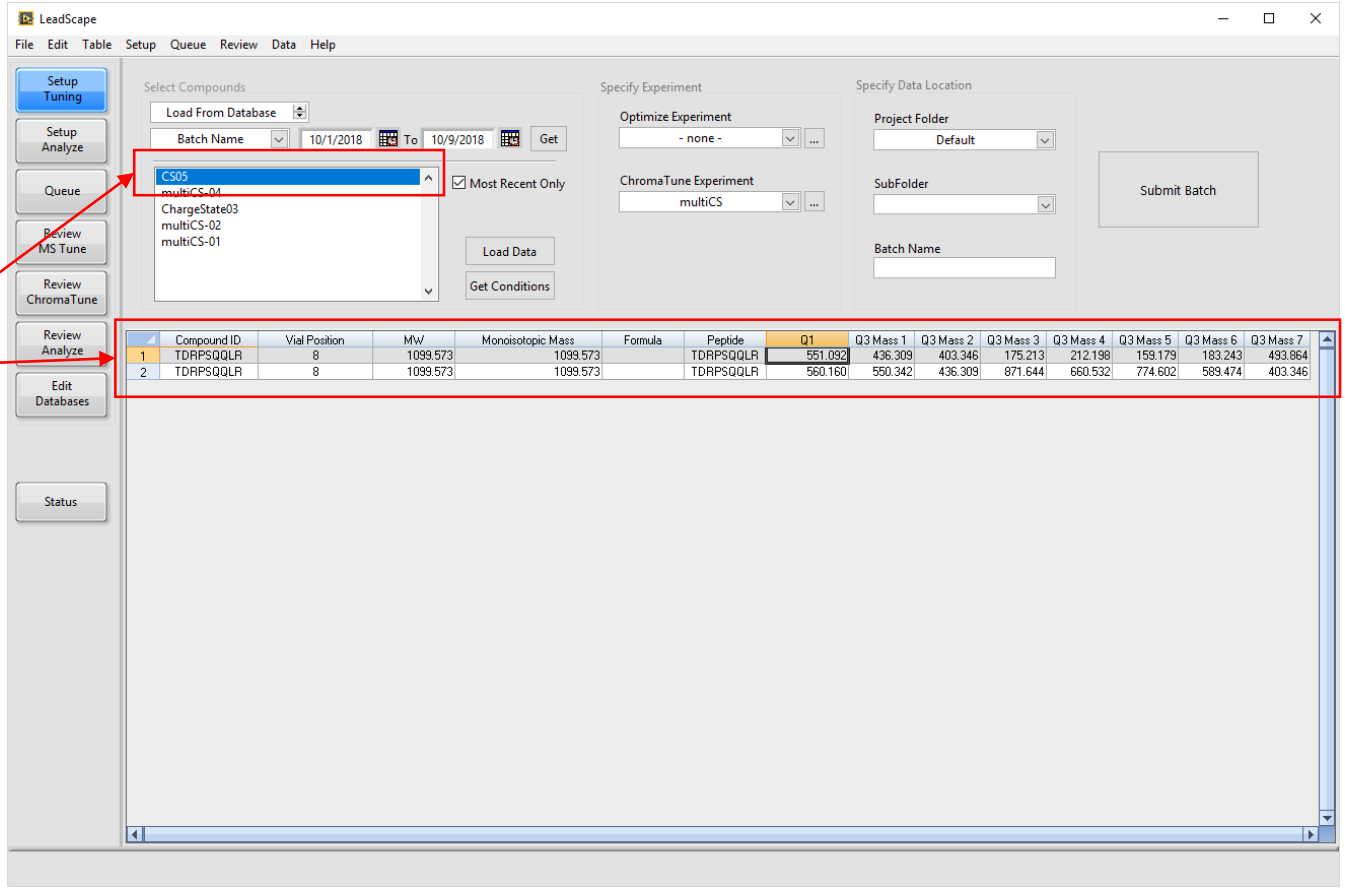
- Inject from the same well, choose a different charge state for each injection
- Make injections of the compound sequential to allow easy review of each injection



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



Review CT Results

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- TBD

Mark Selected Tune

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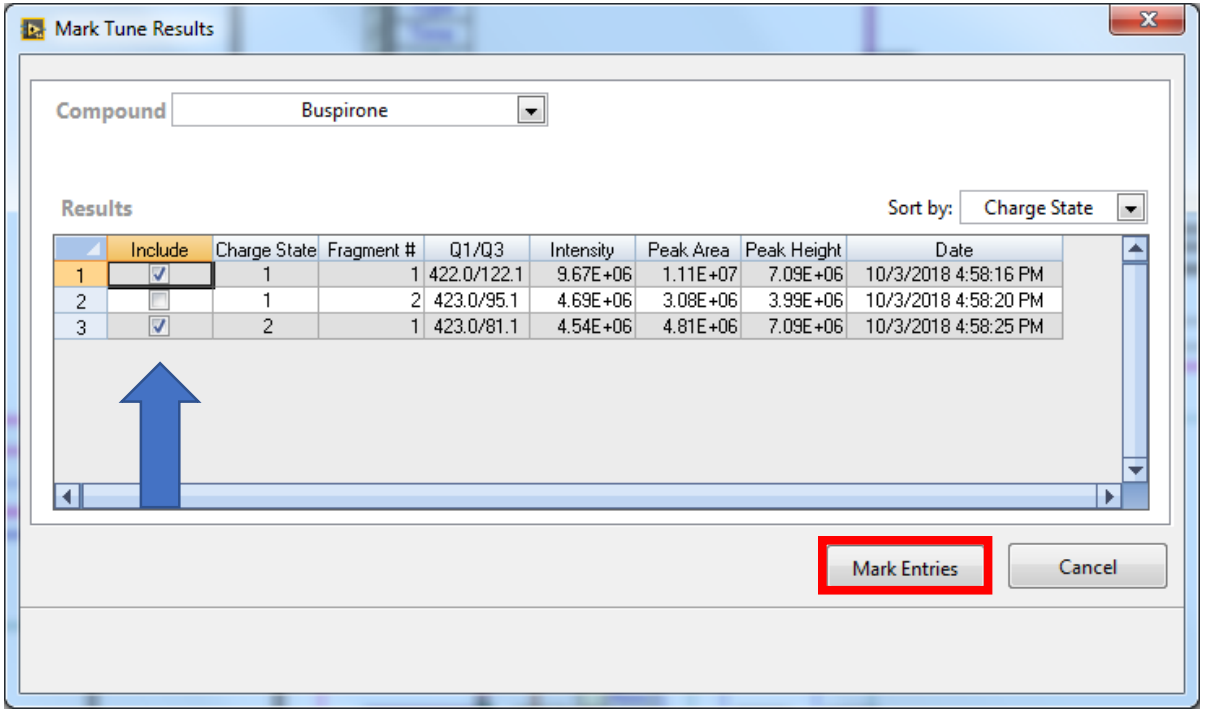
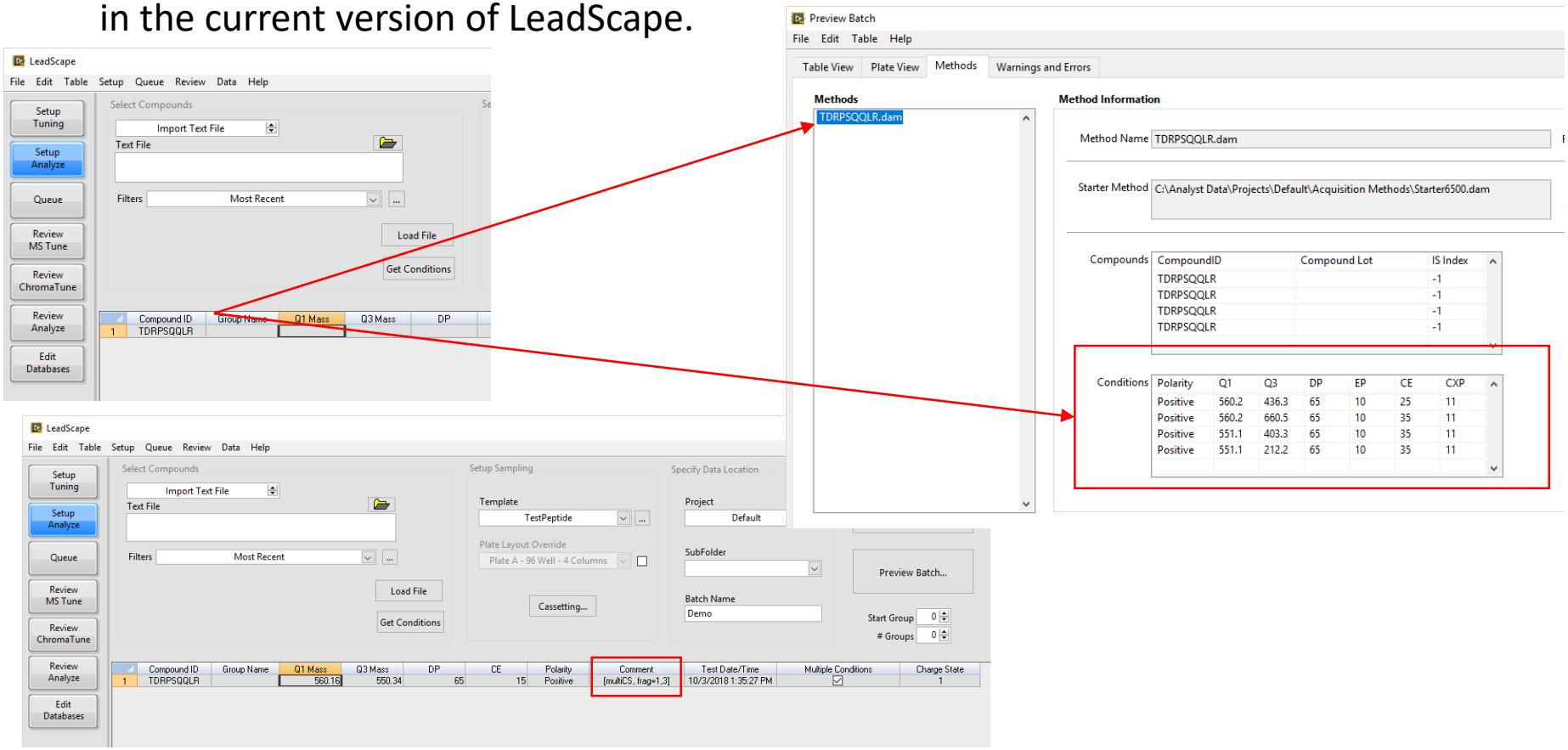
- Select Compound from the list
- Results table will be populated with the MS Tune and CT injection results
- Can sort by any of the table fields to help with selection
- Check Tunes to mark in the database
- Repeat for next compound
- When all compound have been evaluated press Mark Entries to commit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



About

Sound Analytics

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