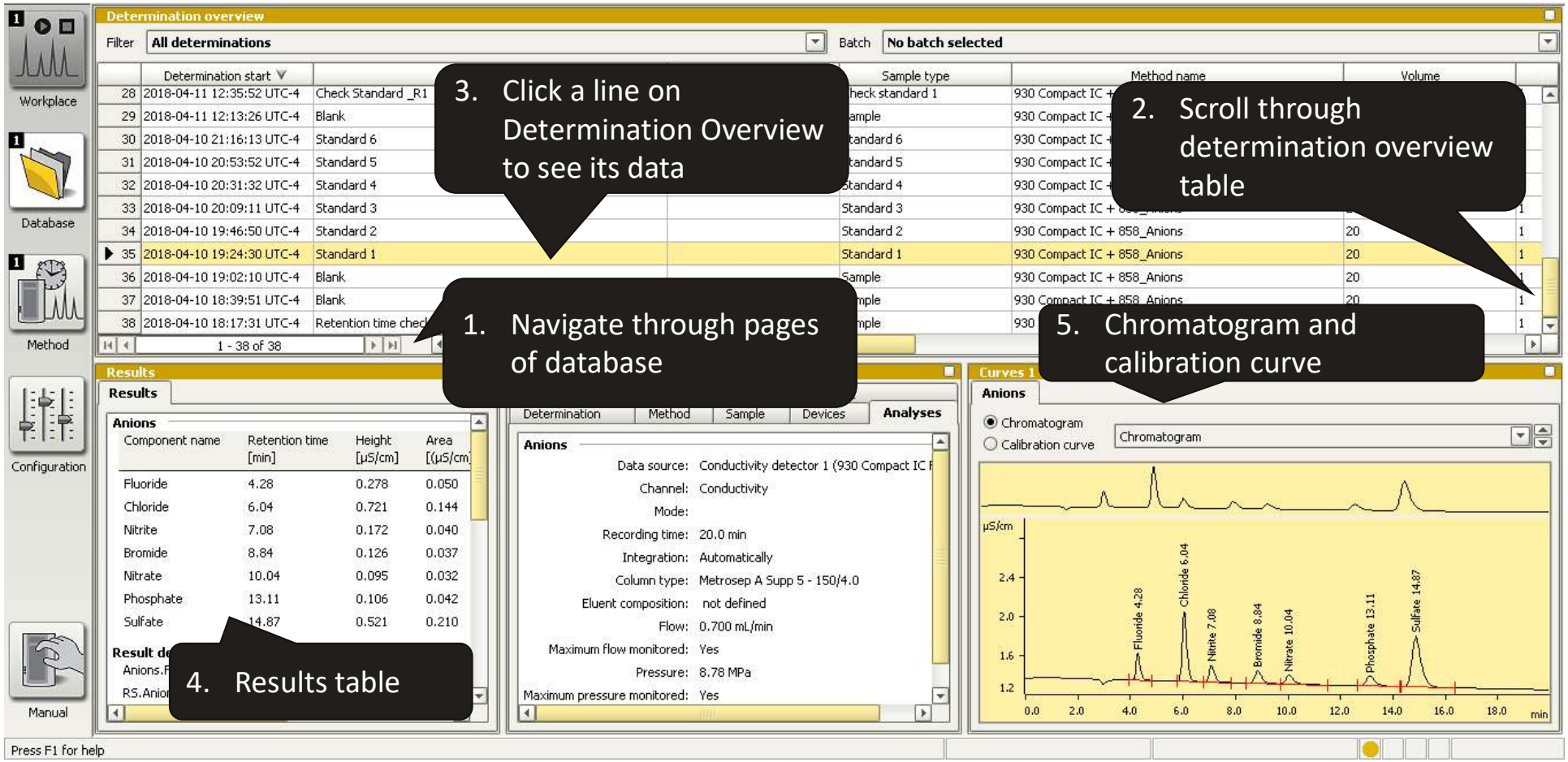
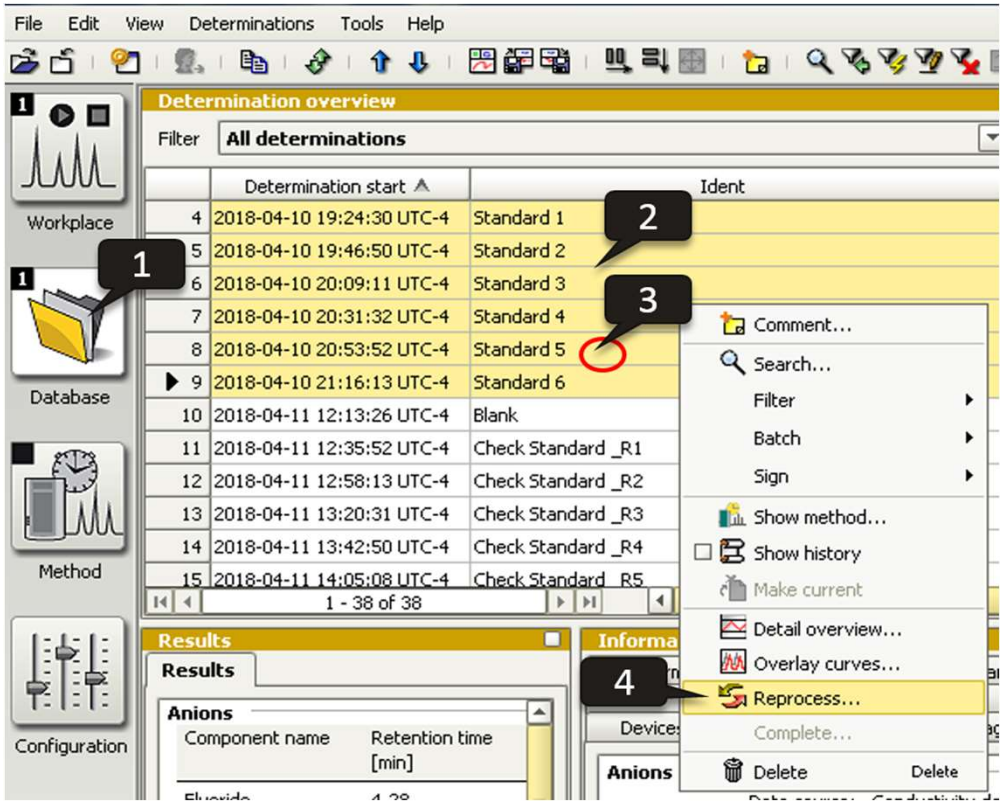
Calibration and Data Evaluation

Database Features

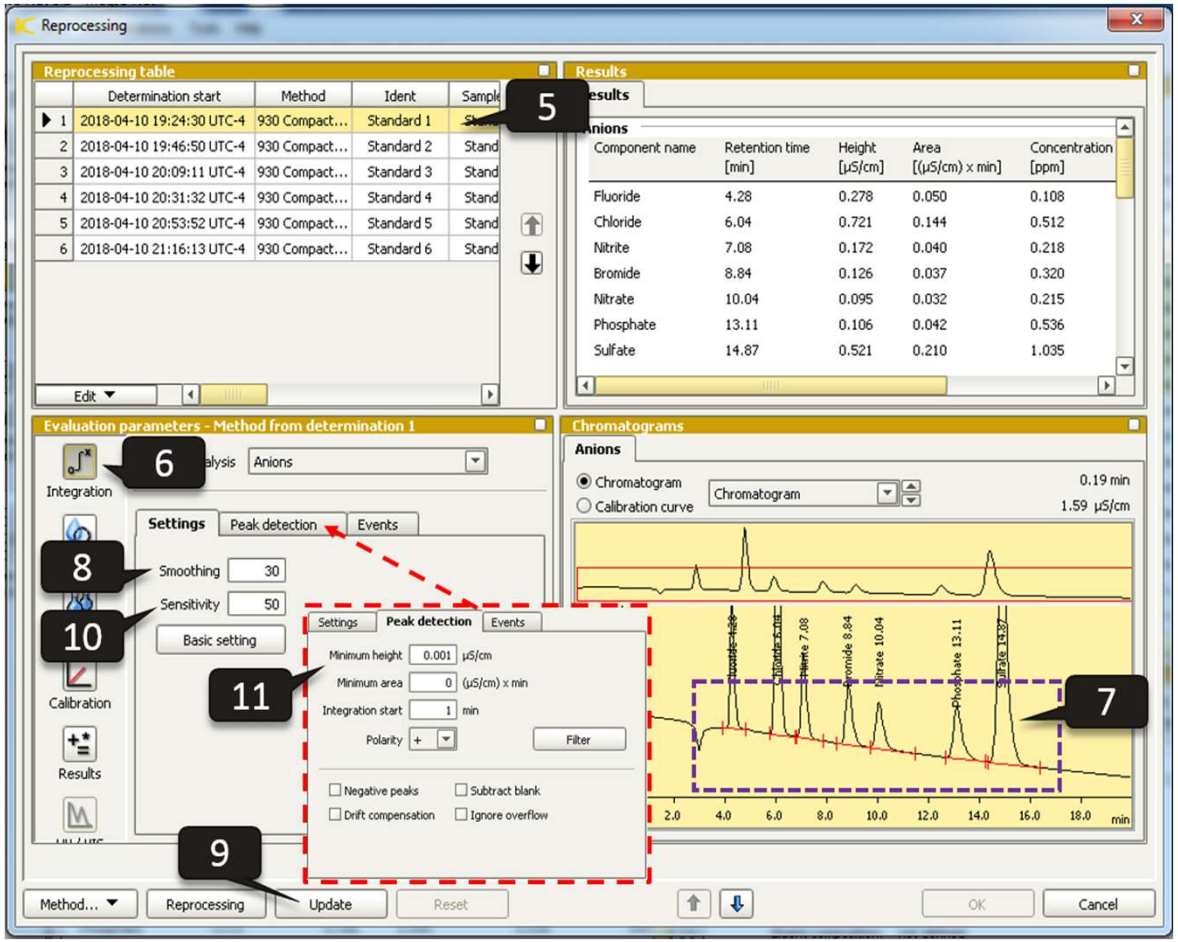


Reprocessing Data



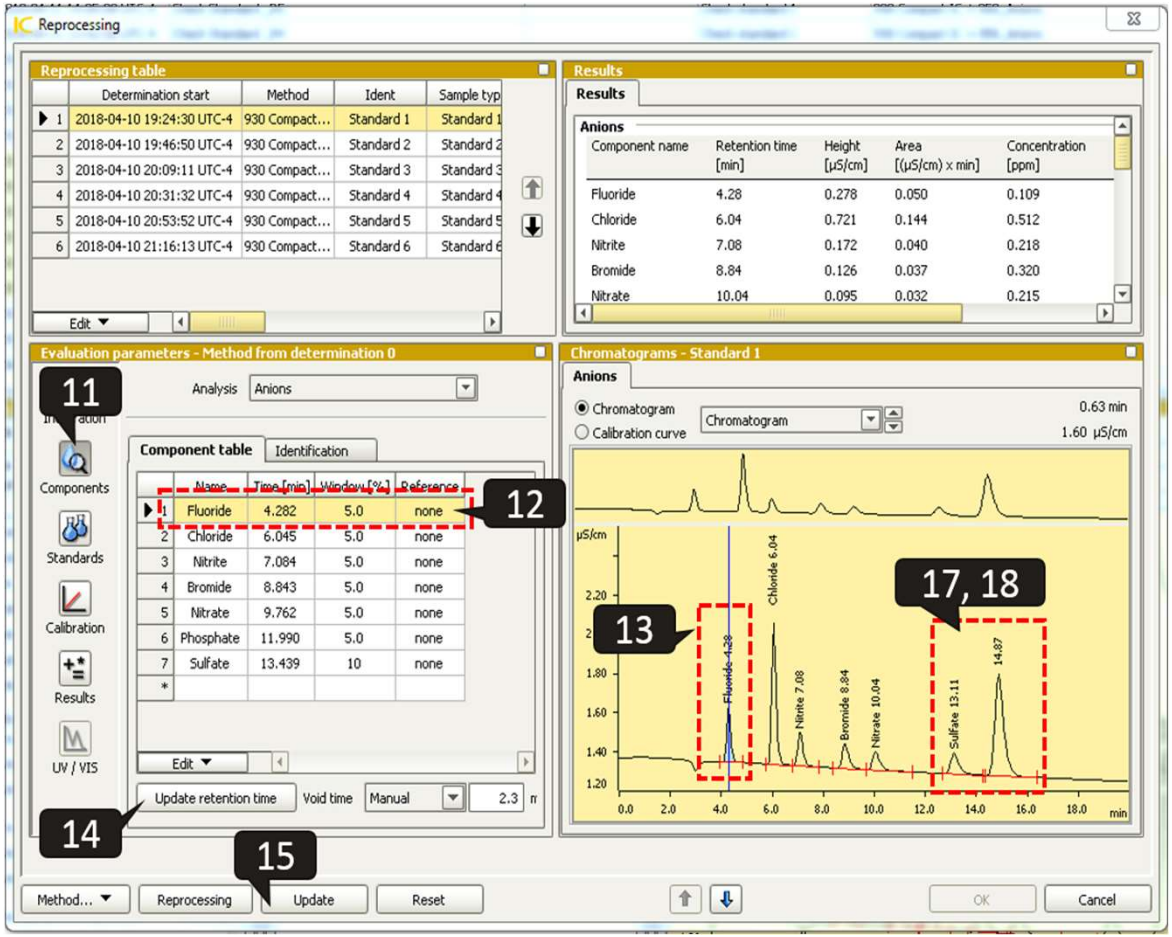
1. Navigate to the Database window of MagIC Net.
2. Select a series of calibration standards that had been previously analyzed
3. Right-click on the selection.
4. Choose Reprocessing in the pop-up menu.

Reprocessing: Peak Integration



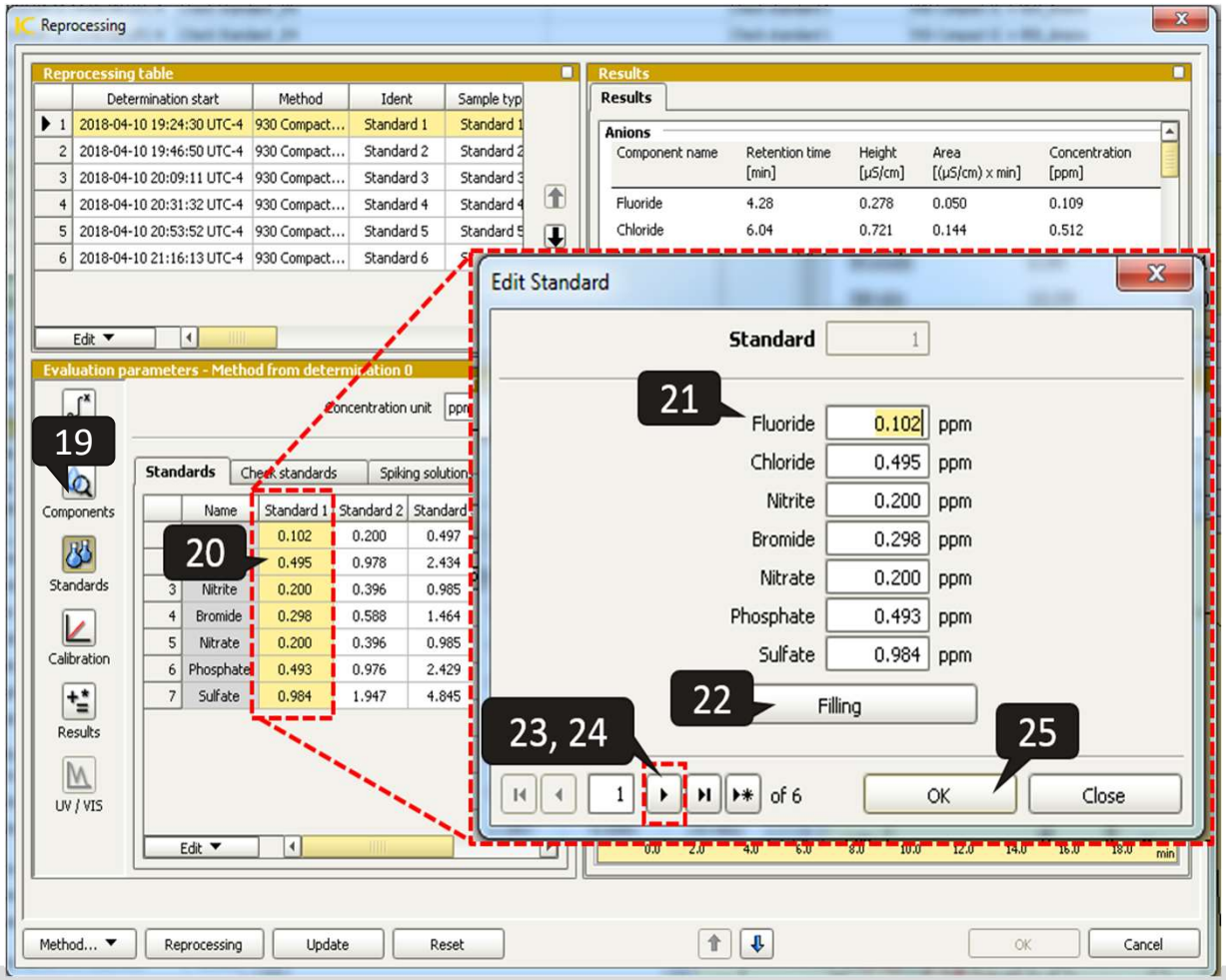
5. In the **Reprocessing table** select the *lowest standard.*
6. Select the **Integration** button under the Evaluation section.
7. Left-click and drag on the Chromatogram to zoom in on the baseline integrations of all the peaks.
8. Increase or decrease **Smoothing** to increase or decrease the integration start and end lines on each peak.
9. Click **Update** after any change to see it applied to the chromatogram.
10. Increase or decrease the **Sensitivity** to have smaller peaks integrated or excluded from integration.
11. Click the **Peak detection** tab to use **Minimum Height** and **Minimum Area** to further adjust the height/area of peaks included or excluded from Integration.

Reprocessing: Component Labeling/ Retention Times



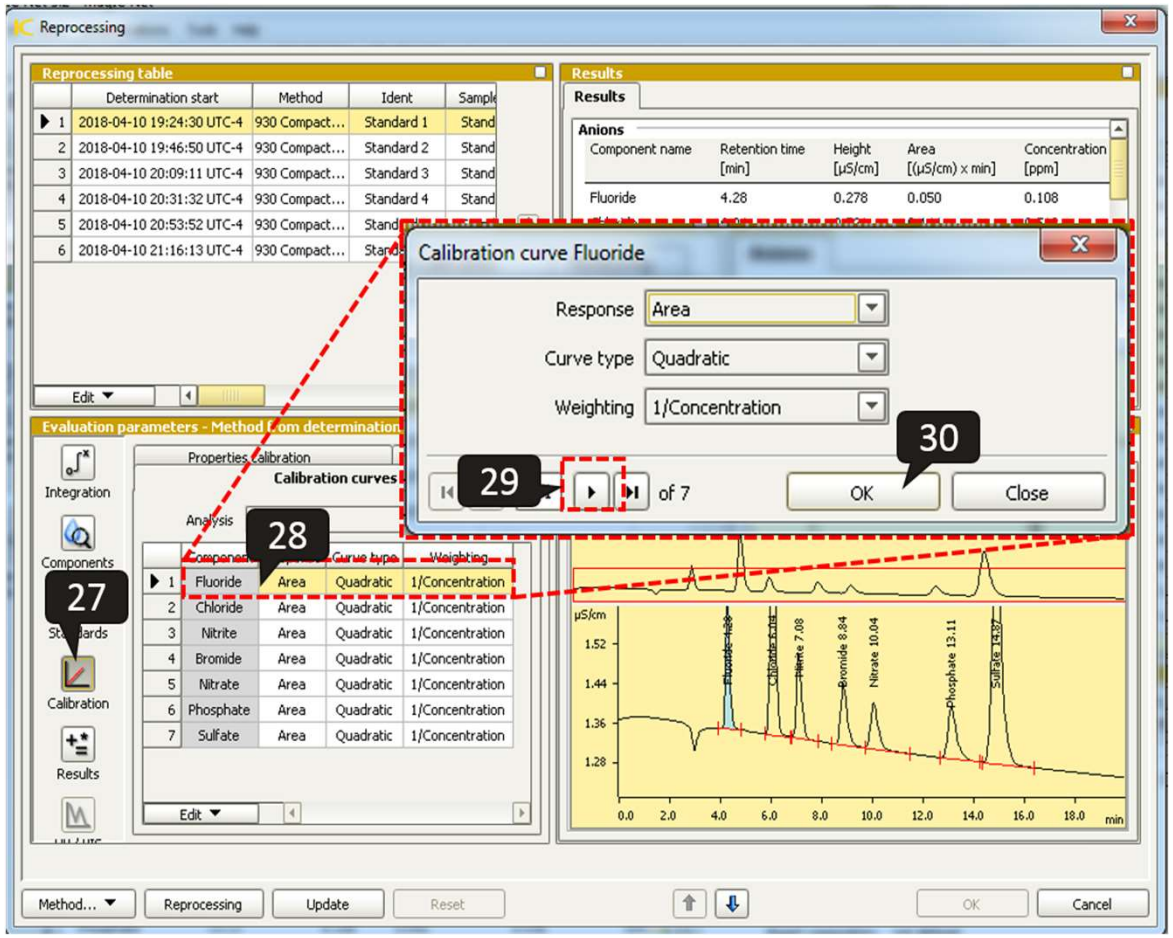
11. In the **Components** button of Evaluation parameters Components labeling and retention times can be updated.
12. Click on the line of the component table for an ion.
13. Left-click on the peak for that ion. This centers the retention time on the apex of the peak.
14. Click the update retention time button. The time on the Component table will be updated.
15. Click the **Update** button to see these changes reflected on the chromatogram.
16. Repeat steps 12-15 for each component ion.
17. If a peak is mislabeled, relabel the unidentified peak first, then hit **Update.**
18. Now update the retention times for the peak which was mislabeled.

Reprocessing: Calibration Concentrations



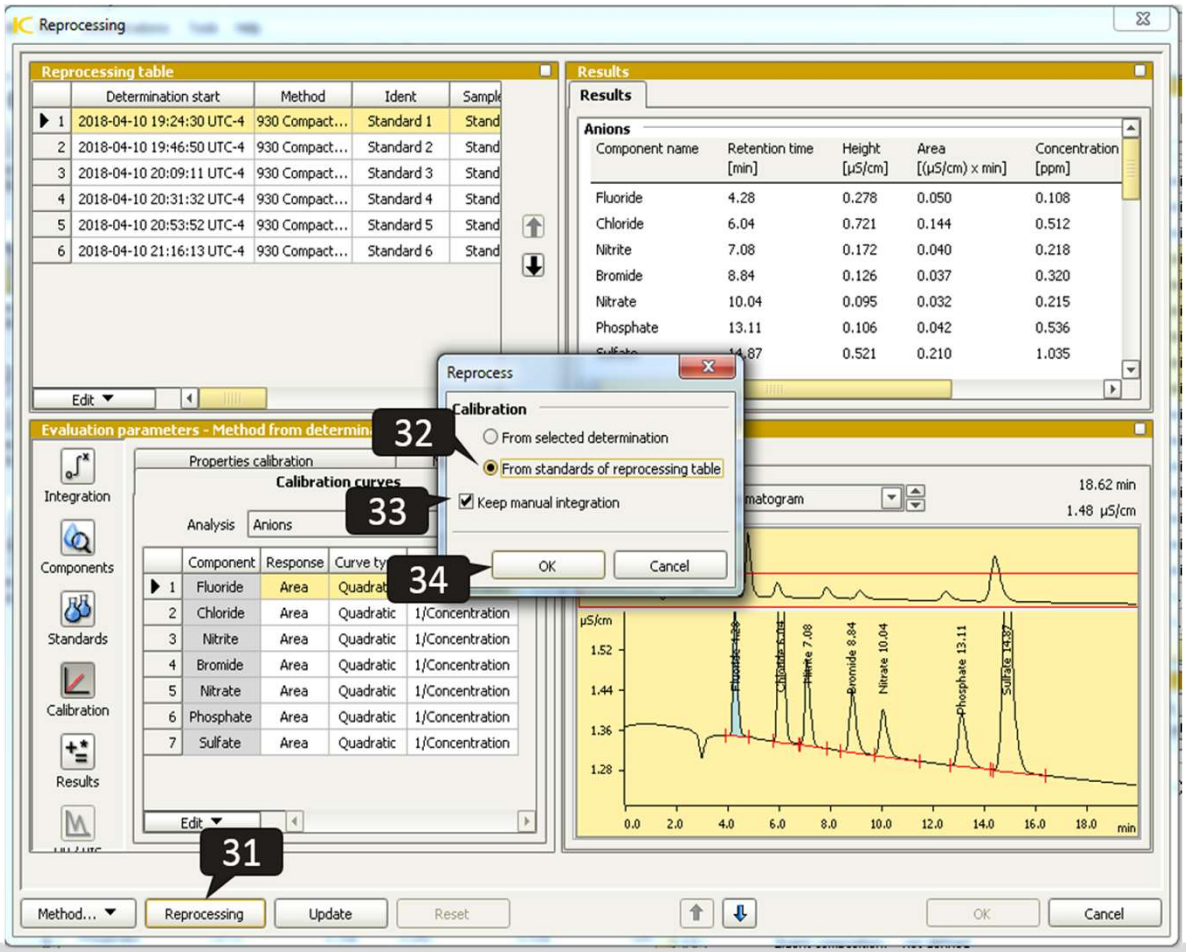
19. Click the Standards button to enter the concentrations of standards, check standards, and matrix spikes.
20. To edit existing concentrations for a particular standard, double-click on that standard to edit.
21. Update the calibration concentrations, pressing the tab key to move from one concentration to the next.
22. If all component ions have the same concentration, enter the value in the first field, then click **Filling.**
23. Use the single arrow to advance through standard levels, and update these standard concentrations.
24. At the end of the list use the single right arrow to add another standard level.
25. Once completed, click the OK button.
26. Repeat steps for Check standards and Spiking Solutions as needed.

Reprocessing: Calibration curves



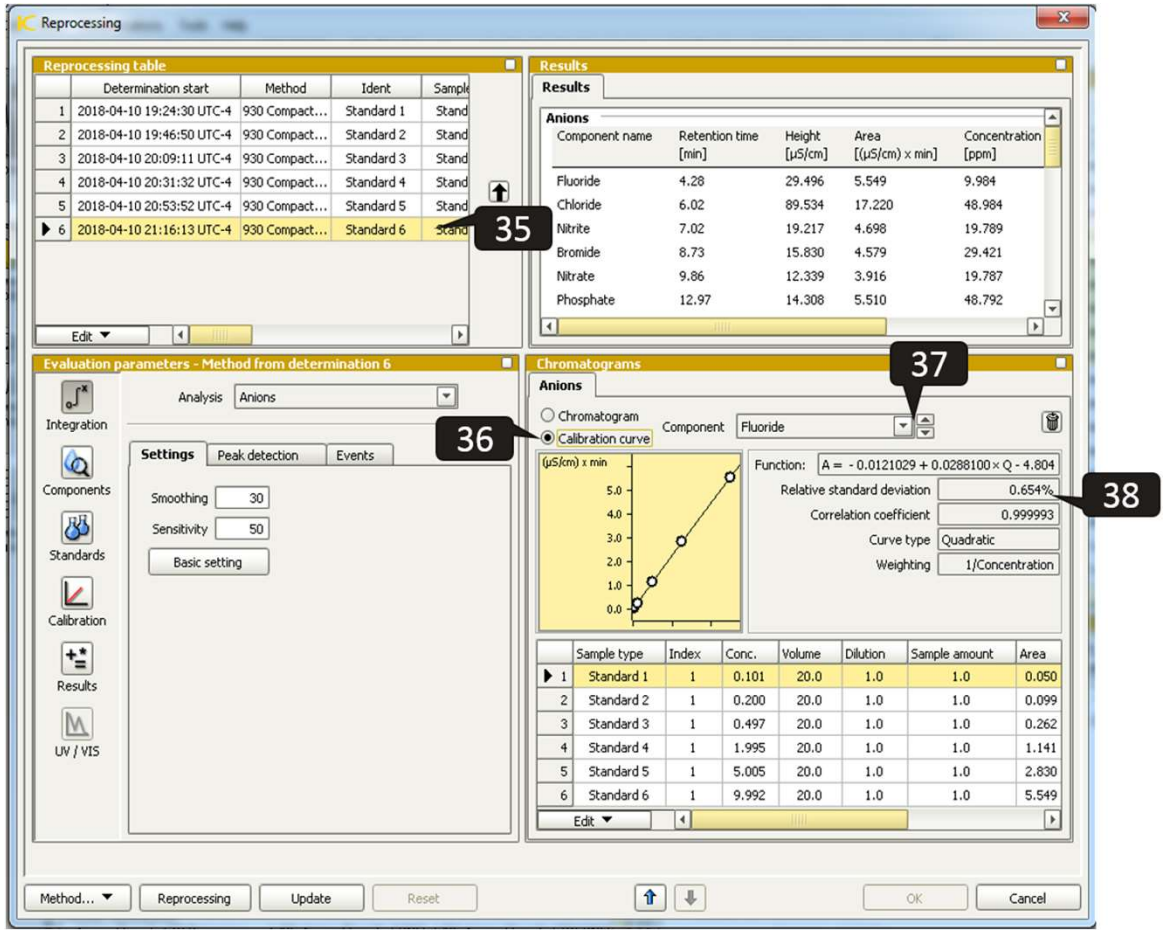
27. To edit the Calibration type utilized, click the Calibration button.
28. Double left-click on the line for a particular ion to edit the Response type used, the Curve type, and the Weighting.
29. Use the single arrows at the bottom of the window to advance to the settings for each ion, making changes as appropriate.
30. Click OK once complete.

Reprocessing: From standards of table



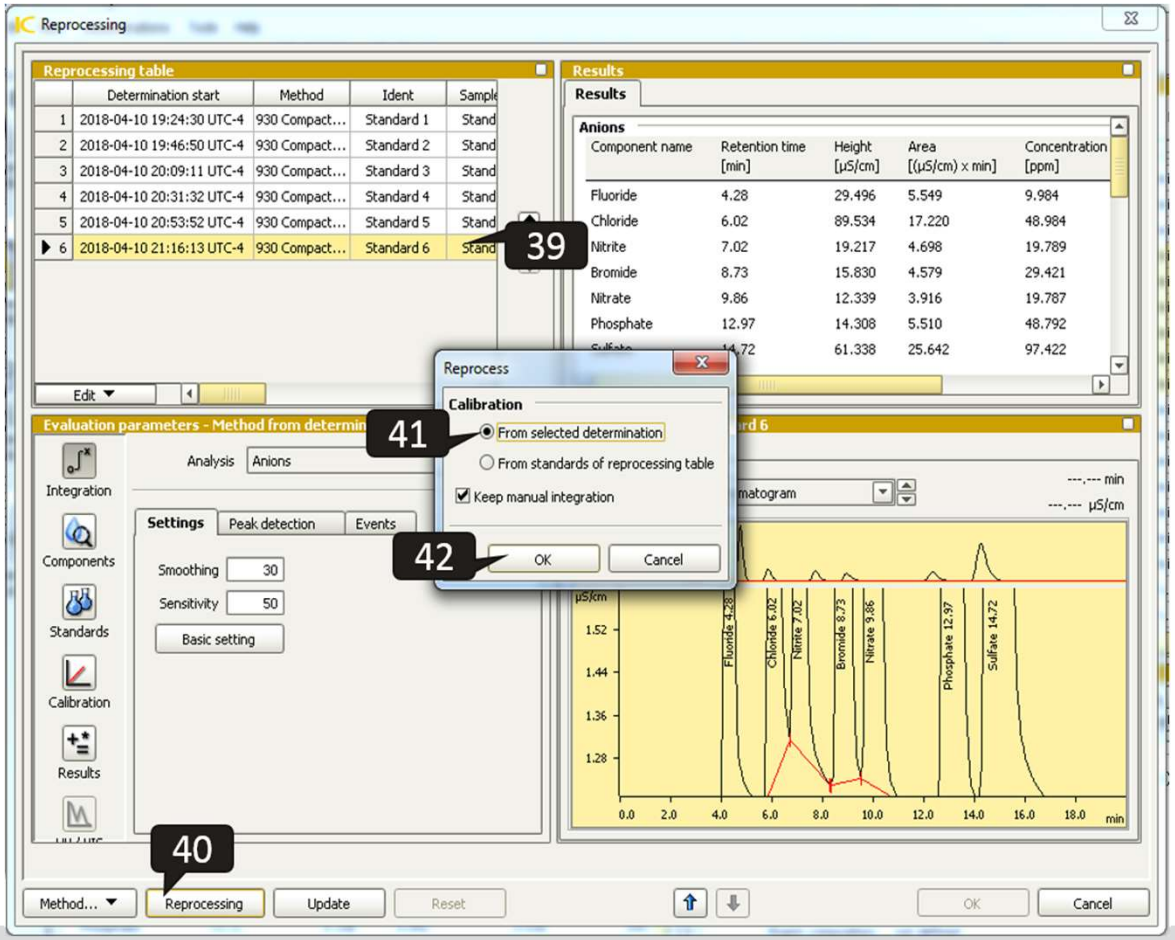
31. To reprocess the changes made to Standard 1 to all other calibration levels, and create a new calibration graph, select **Reprocessing.**
32. Then choose **From standards of reprocessing table**.
33. If you have made manual integration changes, be sure to keep the **Keep manual integration** box checked.
34. Then click **OK.**

Reprocessing: Evaluate calibration curves



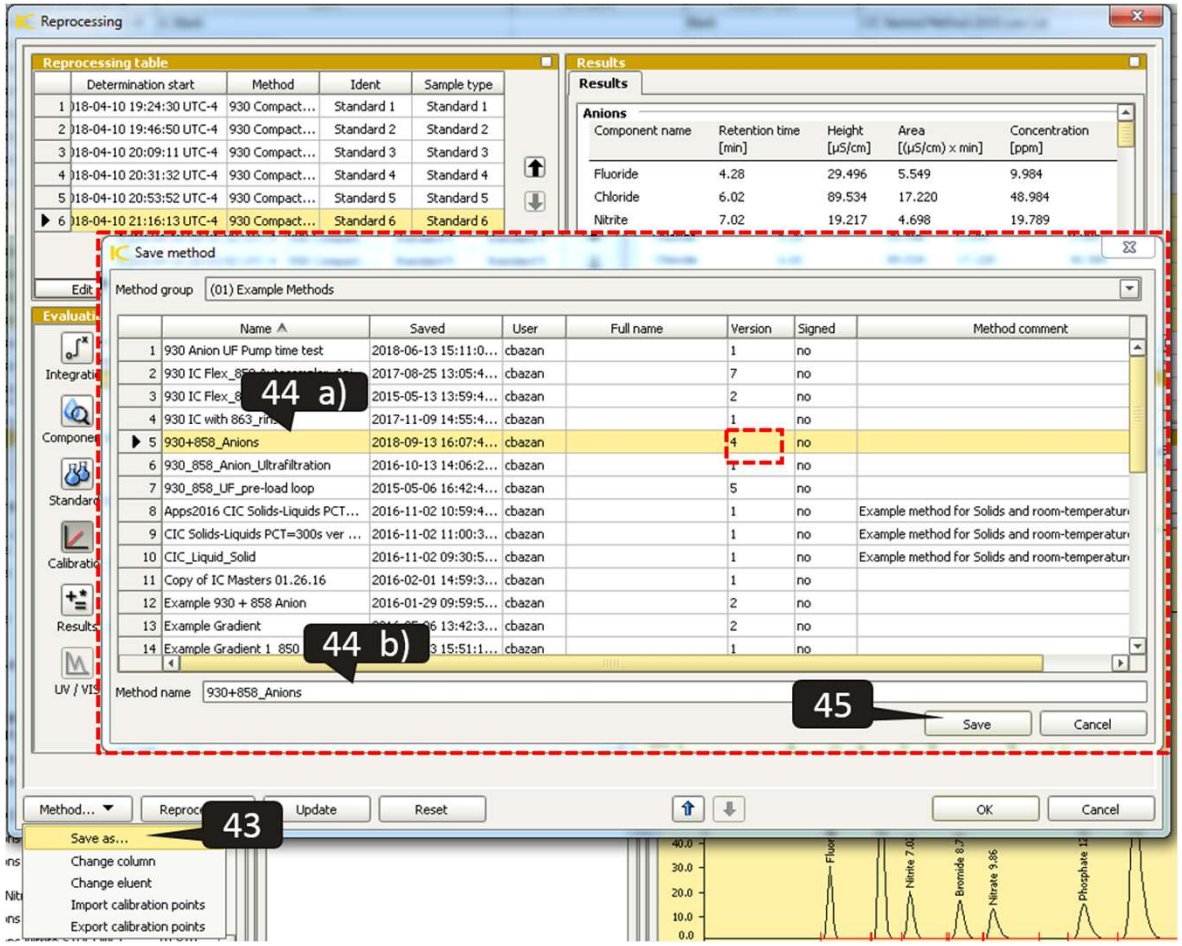
35. Now select the last standard in the Reprocessing table, which is usually the highest calibration standard. All calibration points should be represented in this standard.
36. Click the Calibration Curve button.
37. Use the up and down arrow to scroll through the calibration graph for each analyte, or use the pull-down menu to select the calibration graph for a particular analyte.
38. Evaluate the calibration for Relative Standard Deviation and Correlation Coefficient, based on the criteria of your application.

Reprocessing: From selected determination



39. Highlight the last standard,
40. Click Reprocessing
41. Choose from Selected Determination
42. Press OK. This will apply the full calibration to all standards.

Reprocessing: Save calibration to method



43. Save this new calibration to the method by selecting, **Method → Save as**.

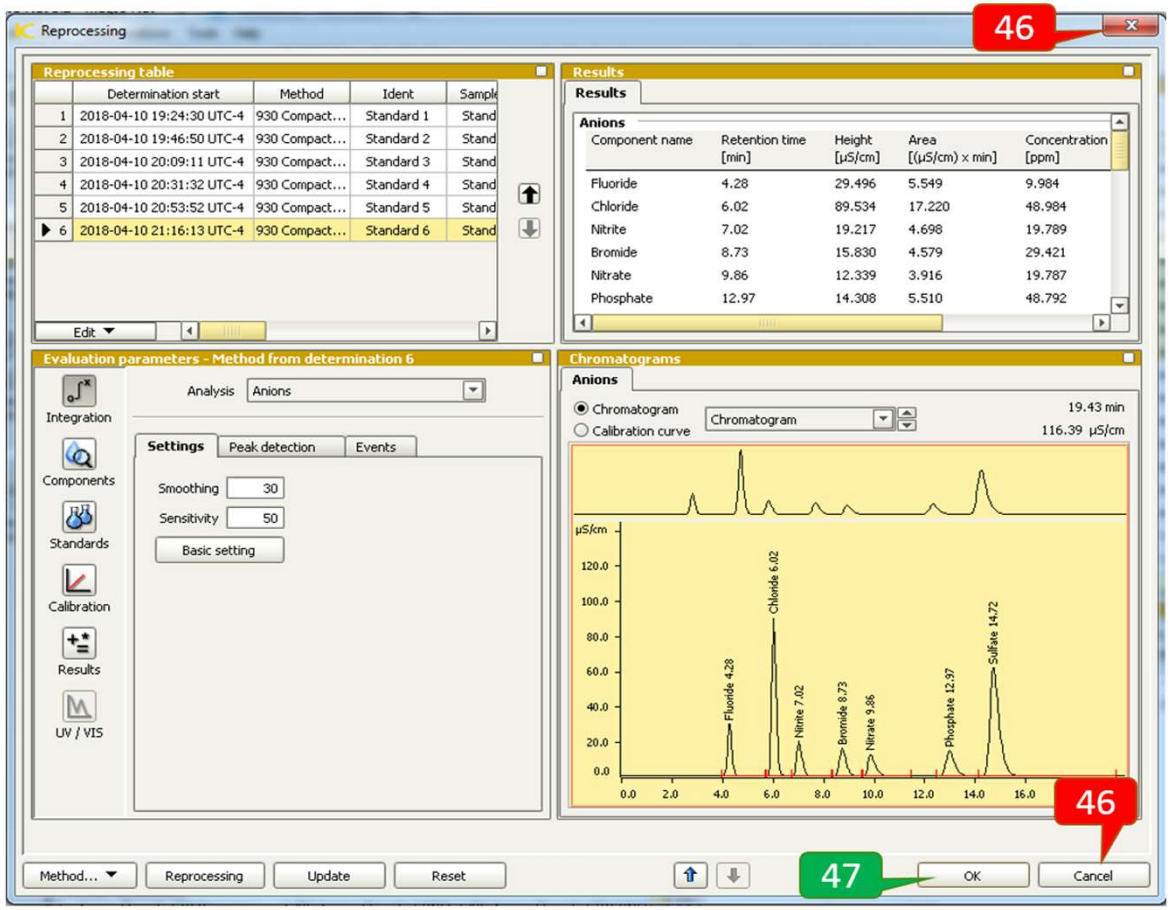
44. Now either:

    a) Select name of the original method. A new version of the method will be generated (new version number). Can revert to previous versions using the History in the Method manager.

    b) Give the method a new name. Be aware if choosing this option the new method name will need to be chosen when running the next Determination series.

45. Click **Save**.

Reprocessing: Save to data

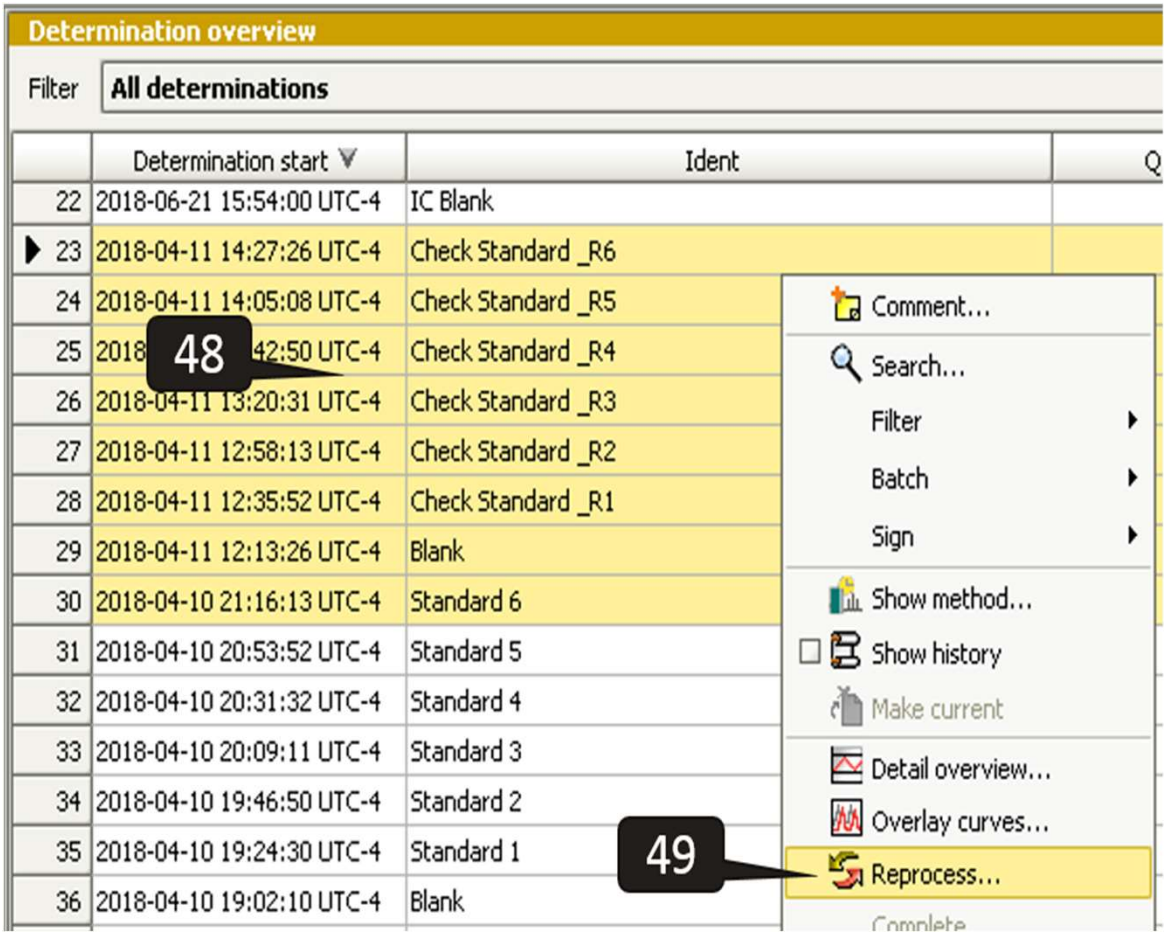


The Reprocess window is a “Sand Box”. If the changes made are not saved to the data, they will be discarded.

46. Clicking the red “**X**” button, or **Cancel**, will discard the changes.

47. Clicking **OK** saves these calibration changes to the determinations shown in the Reprocessing table (e.g. the standards).

Reprocessing: Apply new calibration to samples

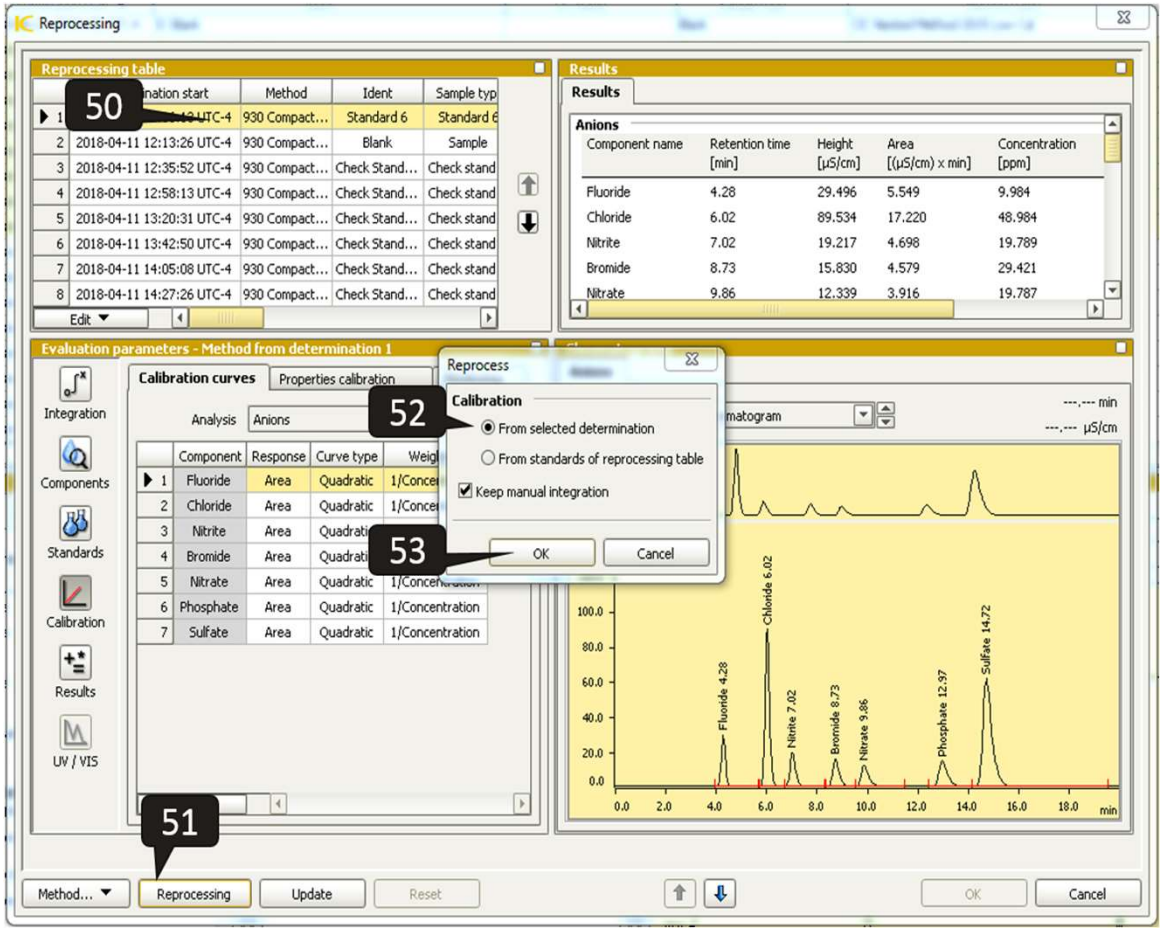


To apply a new calibration generated in reprocessing to a series of samples already run:

48. Highlight the highest calibration standard, then select along with it a block of data to apply it to. It is best to choose blocks of 20 determinations or less at a time to reprocess.

49. Select **Reprocess.**

Reprocessing: Apply new calibration to samples



50. Highlight the calibration standard (contains full calibration curve).
51. Select **Reprocessing**
52. **From Selected determination** (applies full curve to all other determinations in reprocess window).
53. Click **OK** in the Reprocess subwindow.
54. Click **Ok** in the main **Reprocessing** window to save these changes to the data.
55. Repeat steps 48-54 for blocks of ~20 determinations until all data desired has been reprocessed with the appropriate calibration.