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# **Calibration and Data Evaluation**

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# Database Features

The screenshot displays the software interface with five numbered callouts highlighting key features:

- 1. Navigate through pages of database:** Points to the navigation controls at the bottom of the 'Determination overview' table, showing '1 - 38 of 38'.
- 2. Scroll through determination overview table:** Points to the vertical scrollbar on the right side of the 'Determination overview' table.
- 3. Click a line on Determination Overview to see its data:** Points to the highlighted row for 'Standard 1' in the 'Determination overview' table.
- 4. Results table:** Points to the 'Results' section, specifically the 'Anions' table.
- 5. Chromatogram and calibration curve:** Points to the 'Curves' section, showing the 'Chromatogram' view.

**Determination overview table:**

Determination start	Sample type	Method name	Volume
28 2018-04-11 12:35:52 UTC-4	Check standard 1	930 Compact IC +	
29 2018-04-11 12:13:26 UTC-4	Blank	930 Compact IC +	
30 2018-04-10 21:16:13 UTC-4	Standard 6	930 Compact IC +	
31 2018-04-10 20:53:52 UTC-4	Standard 5	930 Compact IC +	
32 2018-04-10 20:31:32 UTC-4	Standard 4	930 Compact IC +	
33 2018-04-10 20:09:11 UTC-4	Standard 3	930 Compact IC +	
34 2018-04-10 19:46:50 UTC-4	Standard 2	930 Compact IC + 858_Anions	20
35 2018-04-10 19:24:30 UTC-4	Standard 1	930 Compact IC + 858_Anions	20
36 2018-04-10 19:02:10 UTC-4	Sample	930 Compact IC + 858_Anions	20
37 2018-04-10 18:39:51 UTC-4	Sample	930 Compact IC + 858_Anions	20
38 2018-04-10 18:17:31 UTC-4	Sample	930 Compact IC + 858_Anions	20

**Results - Anions table:**

Component name	Retention time [min]	Height [ $\mu\text{S}/\text{cm}$ ]	Area [ $(\mu\text{S}/\text{cm})$ ]
Fluoride	4.28	0.278	0.050
Chloride	6.04	0.721	0.144
Nitrite	7.08	0.172	0.040
Bromide	8.84	0.126	0.037
Nitrate	10.04	0.095	0.032
Phosphate	13.11	0.106	0.042
Sulfate	14.87	0.521	0.210

**Analyses - Anions:**

- Data source: Conductivity detector 1 (930 Compact IC)
- Channel: Conductivity
- Mode:
- Recording time: 20.0 min
- Integration: Automatically
- Column type: Metrosep A Supp 5 - 150/4.0
- Eluent composition: not defined
- Flow: 0.700 mL/min
- Maximum flow monitored: Yes
- Pressure: 8.78 MPa
- Maximum pressure monitored: Yes

**Curves - Anions:**

- Selected: Chromatogram
- Y-axis:  $\mu\text{S}/\text{cm}$
- X-axis: min
- Peaks labeled: Fluoride 4.28, Chloride 6.04, Nitrite 7.08, Bromide 8.84, Nitrate 10.04, Phosphate 13.11, Sulfate 14.87

# Reprocessing Data

The screenshot shows the MagIC Net software interface. The main window is titled "Determination overview" and contains a table of determinations. The table has columns for "Determination start" and "Ident". A right-click context menu is open over the table, with the "Reprocess..." option highlighted. Numbered callouts (1-4) indicate the steps:

1. Clicking the "Database" icon in the left sidebar.
2. Selecting a row in the table.
3. Right-clicking on the selected row.
4. Clicking the "Reprocess..." option in the context menu.

	Determination start	Ident
4	2018-04-10 19:24:30 UTC-4	Standard 1
5	2018-04-10 19:46:50 UTC-4	Standard 2
6	2018-04-10 20:09:11 UTC-4	Standard 3
7	2018-04-10 20:31:32 UTC-4	Standard 4
8	2018-04-10 20:53:52 UTC-4	Standard 5
9	2018-04-10 21:16:13 UTC-4	Standard 6
10	2018-04-11 12:13:26 UTC-4	Blank
11	2018-04-11 12:35:52 UTC-4	Check Standard _R1
12	2018-04-11 12:58:13 UTC-4	Check Standard _R2
13	2018-04-11 13:20:31 UTC-4	Check Standard _R3
14	2018-04-11 13:42:50 UTC-4	Check Standard _R4
15	2018-04-11 14:05:08 UTC-4	Check Standard _R5

The context menu options are: Comment..., Search..., Filter, Batch, Sign, Show method..., Show history, Make current, Detail overview..., Overlay curves..., Reprocess..., Complete..., and Delete.

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

The screenshot shows the 'Reprocessing' software interface. The 'Reprocessing table' lists six samples. The 'Results' table shows the following data:

Component name	Retention time [min]	Height [ $\mu\text{S}/\text{cm}$ ]	Area [ $(\mu\text{S}/\text{cm}) \times \text{min}$ ]	Concentration [ppm]
Fluoride	4.28	0.278	0.050	0.108
Chloride	6.04	0.721	0.144	0.512
Nitrite	7.08	0.172	0.040	0.218
Bromide	8.84	0.126	0.037	0.320
Nitrate	10.04	0.095	0.032	0.215
Phosphate	13.11	0.106	0.042	0.536
Sulfate	14.87	0.521	0.210	1.035

The 'Evaluation parameters' section shows 'Anions' analysis with 'Peak detection' settings. The 'Chromatograms' section shows a chromatogram with peaks labeled: Fluoride 4.28, Chloride 6.04, Nitrite 7.08, Bromide 8.84, Nitrate 10.04, Phosphate 13.11, and Sulfate 14.87. A red dashed box highlights the 'Peak detection' settings, and a blue dashed box highlights the chromatogram peaks.

- In the **Reprocessing table** select the *lowest standard*.
- Select the **Integration** button under the Evaluation section.
- Left-click and drag on the Chromatogram to zoom in on the baseline integrations of all the peaks.
- Increase or decrease **Smoothing** to increase or decrease the integration start and end lines on each peak.
- Click **Update** after any change to see it applied to the chromatogram.
- Increase or decrease the **Sensitivity** to have smaller peaks integrated or excluded from integration.
- 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

The screenshot displays the 'Reprocessing' software interface with several key sections:

- Reprocessing table:** A table listing determination start times, methods, identifiers, and sample types.
- Results:** A table showing anions with their retention times, heights, areas, and concentrations.
- Evaluation parameters - Method from determination 0:** A section for analysis parameters, including a 'Component table'.
- Chromatograms - Standard 1:** A chromatogram plot showing peaks for various anions.

Numbered callouts (11-18) indicate the steps for reprocessing:

- 11:** Points to the 'Anions' dropdown menu in the 'Evaluation parameters' section.
- 12:** Points to the first row (Fluoride) in the 'Component table'.
- 13:** Points to the peak for Fluoride in the chromatogram.
- 14:** Points to the 'Update retention time' button.
- 15:** Points to the 'Update' button at the bottom of the interface.
- 17, 18:** Points to a mislabeled peak (Sulfate) in the chromatogram.

Determination start	Method	Ident	Sample type
2018-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Standard 1
2018-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Standard 2
2018-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Standard 3
2018-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Standard 4
2018-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Standard 5
2018-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Standard 6

Component name	Retention time [min]	Height [µS/cm]	Area [(µS/cm) × min]	Concentration [ppm]
Fluoride	4.28	0.278	0.050	0.109
Chloride	6.04	0.721	0.144	0.512
Nitrite	7.08	0.172	0.040	0.218
Bromide	8.84	0.126	0.037	0.320
Nitrate	10.04	0.095	0.032	0.215

Name	Time [min]	Window [%]	Reference
1 Fluoride	4.282	5.0	none
2 Chloride	6.045	5.0	none
3 Nitrite	7.084	5.0	none
4 Bromide	8.843	5.0	none
5 Nitrate	9.762	5.0	none
6 Phosphate	11.990	5.0	none
7 Sulfate	13.439	10	none
*			

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

The screenshot shows the 'Reprocessing' software interface. The 'Edit Standard' dialog box is open, displaying a list of components and their concentrations. The 'Standards' table in the background is as follows:

Name	Standard 1	Standard 2	Standard 3
1	0.102	0.200	0.497
2	0.495	0.978	2.434
3 Nitrite	0.200	0.396	0.985
4 Bromide	0.298	0.588	1.464
5 Nitrate	0.200	0.396	0.985
6 Phosphate	0.493	0.976	2.429
7 Sulfate	0.984	1.947	4.845

The 'Edit Standard' dialog box shows the following components and concentrations:

Fluoride	0.102	ppm
Chloride	0.495	ppm
Nitrite	0.200	ppm
Bromide	0.298	ppm
Nitrate	0.200	ppm
Phosphate	0.493	ppm
Sulfate	0.984	ppm

The 'Filling' button is visible at the bottom of the dialog box. The 'OK' button is also visible.

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

The screenshot displays the 'Reprocessing' software interface. The 'Reprocessing table' shows a list of samples. The 'Results' section shows a table of anions. The 'Calibration curves' table lists components and their calibration parameters. A 'Calibration curve Fluoride' dialog box is open, showing settings for Response, Curve type, and Weighting. A chromatogram is visible at the bottom right.

Determination start	Method	Ident	Sample
2018-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Stand
2018-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Stand
2018-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Stand
2018-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Stand
2018-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Stand
2018-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Stand

Component name	Retention time [min]	Height [μS/cm]	Area [(μS/cm) × min]	Concentration [ppm]
Fluoride	4.28	0.278	0.050	0.108

Component	Response	Curve type	Weighting
1 Fluoride	Area	Quadratic	1/Concentration
2 Chloride	Area	Quadratic	1/Concentration
3 Nitrite	Area	Quadratic	1/Concentration
4 Bromide	Area	Quadratic	1/Concentration
5 Nitrate	Area	Quadratic	1/Concentration
6 Phosphate	Area	Quadratic	1/Concentration
7 Sulfate	Area	Quadratic	1/Concentration

Calibration curve Fluoride

Response: Area  
Curve type: Quadratic  
Weighting: 1/Concentration

29 of 7

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Chromatogram showing peaks for Fluoride (4.28 min), Chloride (7.08 min), Bromide (8.84 min), Nitrate (10.04 min), Phosphate (13.11 min), and Sulfate (14.87 min).

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

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Determination start	Method	Ident	Sample
2018-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Stand
2018-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Stand
2018-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Stand
2018-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Stand
2018-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Stand
2018-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Stand

Component name	Retention time [min]	Height [µS/cm]	Area [(µS/cm) × min]	Concentration [ppm]
Fluoride	4.28	0.278	0.050	0.108
Chloride	6.04	0.721	0.144	0.512
Nitrite	7.08	0.172	0.040	0.218
Bromide	8.84	0.126	0.037	0.320
Nitrate	10.04	0.095	0.032	0.215
Phosphate	13.11	0.106	0.042	0.536
Sulfate	14.87	0.521	0.210	1.035

Component	Response	Curve type
1 Fluoride	Area	Quadratic
2 Chloride	Area	Quadratic
3 Nitrite	Area	Quadratic
4 Bromide	Area	Quadratic
5 Nitrate	Area	Quadratic
6 Phosphate	Area	Quadratic
7 Sulfate	Area	Quadratic

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

The screenshot shows the 'Reprocessing' software interface. The 'Reprocessing table' panel contains a table with columns: Determination start, Method, Ident, and Sample. The 'Results' panel shows a table of 'Anions' with columns: Component name, Retention time [min], Height [µS/cm], Area [(µS/cm) × min], and Concentration [ppm]. The 'Evaluation parameters - Method from determination 6' panel has tabs for 'Settings', 'Peak detection', and 'Events'. The 'Chromatograms' panel shows a 'Calibration curve' graph for 'Fluoride' with a function:  $A = -0.0121029 + 0.0288100 \times Q - 4.804$ . Below the graph is a table with columns: Sample type, Index, Conc., Volume, Dilution, Sample amount, and Area.

Determination start	Method	Ident	Sample
2018-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Stand
2018-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Stand
2018-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Stand
2018-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Stand
2018-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Stand
2018-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Stand

Component name	Retention time [min]	Height [µS/cm]	Area [(µS/cm) × min]	Concentration [ppm]
Fluoride	4.28	29.496	5.549	9.984
Chloride	6.02	89.534	17.220	48.984
Nitrite	7.02	19.217	4.698	19.789
Bromide	8.73	15.830	4.579	29.421
Nitrate	9.86	12.339	3.916	19.787
Phosphate	12.97	14.308	5.510	48.792

Sample type	Index	Conc.	Volume	Dilution	Sample amount	Area
Standard 1	1	0.101	20.0	1.0	1.0	0.050
Standard 2	1	0.200	20.0	1.0	1.0	0.099
Standard 3	1	0.497	20.0	1.0	1.0	0.262
Standard 4	1	1.995	20.0	1.0	1.0	1.141
Standard 5	1	5.005	20.0	1.0	1.0	2.830
Standard 6	1	9.992	20.0	1.0	1.0	5.549

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

The screenshot shows the 'Reprocessing' software interface. The 'Reprocessing table' lists six determinations, with the last one (Standard 6) highlighted. The 'Results' table shows data for various anions. The 'Evaluation parameters' section is visible, and a 'Reprocess' dialog box is open, showing the 'Calibration' options. The 'From selected determination' option is selected, and the 'OK' button is highlighted.

Determination start	Method	Ident	Sample
2018-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Stand
2018-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Stand
2018-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Stand
2018-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Stand
2018-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Stand
2018-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Stand

Component name	Retention time [min]	Height [µS/cm]	Area [(µS/cm) × min]	Concentration [ppm]
Fluoride	4.28	29.496	5.549	9.984
Chloride	6.02	89.534	17.220	48.984
Nitrite	7.02	19.217	4.698	19.789
Bromide	8.73	15.830	4.579	29.421
Nitrate	9.86	12.339	3.916	19.787
Phosphate	12.97	14.308	5.510	48.792
Sulfate	14.72	61.338	25.642	97.422

Reprocess dialog box options:

- From selected determination
- From standards of reprocessing table
- Keep manual integration

Chromatogram peaks (Retention time [min]):

- Fluoride 4.28
- Chloride 6.02
- Nitrite 7.02
- Bromide 8.73
- Nitrate 9.86
- Phosphate 12.97
- Sulfate 14.72

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

**Reprocessing table**

Determination start	Method	Ident	Sample type
1 18-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Standard 1
2 18-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Standard 2
3 18-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Standard 3
4 18-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Standard 4
5 18-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Standard 5
6 18-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Standard 6

**Results**

Component name	Retention time [min]	Height [μS/cm]	Area [(μS/cm) x min]	Concentration [ppm]
Fluoride	4.28	29.496	5.549	9.984
Chloride	6.02	89.534	17.220	48.984
Nitrite	7.02	19.217	4.698	19.789

**Save method**

Method group: (01) Example Methods

Name	Saved	User	Full name	Version	Signed	Method comment
1 930 Anion UF Pump time test	2018-06-13 15:11:0...	cbazan		1	no	
2 930 IC Flex_858...	2017-08-25 13:05:4...	cbazan		7	no	
3 930 IC Flex_8...	2015-05-13 13:59:4...	cbazan		2	no	
4 930 IC with 863_rin...	2017-11-09 14:55:4...	cbazan		1	no	
5 930+858_Anions	2018-09-13 16:07:4...	cbazan		1	no	
6 930_858_Anion_Ultrafiltration	2016-10-13 14:06:2...	cbazan		1	no	
7 930_858_UF_pre-load loop	2015-05-06 16:42:4...	cbazan		5	no	
8 Apps2016 CIC Solids-Liquids PCT...	2016-11-02 10:59:4...	cbazan		1	no	Example method for Solids and room-temperat...
9 CIC Solids-Liquids PCT=300s ver ...	2016-11-02 11:00:3...	cbazan		1	no	Example method for Solids and room-temperat...
10 CIC_Liquid_Solid	2016-11-02 09:30:5...	cbazan		1	no	
11 Copy of IC Masters 01.26.16	2016-02-01 14:59:3...	cbazan		1	no	
12 Example 930 + 858 Anion	2016-01-29 09:59:5...	cbazan		2	no	
13 Example Gradient	2016-02-06 13:42:3...	cbazan		2	no	
14 Example Gradient 1 850	2016-02-06 13:51:1...	cbazan		1	no	

Method name: 930+858\_Anions

**Save as...**

- Change column
- Change eluent
- Import calibration points
- Export calibration points

**43** Save as... **44 a** 930+858\_Anions **44 b** Method name **45** Save

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

44. Now either:

- 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.
- 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 screenshot displays the 'Reprocessing' software interface. It features several panels: 'Reprocessing table' with a list of determinations, 'Results' showing a table of anion data, 'Evaluation parameters - Method from determination 6' with settings for integration and components, and 'Chromatograms' showing a chromatogram plot. A red callout '46' points to the 'X' button in the top right corner. Another red callout '46' points to the 'OK' button at the bottom right. A green callout '47' points to the 'OK' button at the bottom center.

Determination start	Method	Ident	Sample
2018-04-10 19:24:30 UTC-4	930 Compact...	Standard 1	Stand
2018-04-10 19:46:50 UTC-4	930 Compact...	Standard 2	Stand
2018-04-10 20:09:11 UTC-4	930 Compact...	Standard 3	Stand
2018-04-10 20:31:32 UTC-4	930 Compact...	Standard 4	Stand
2018-04-10 20:53:52 UTC-4	930 Compact...	Standard 5	Stand
2018-04-10 21:16:13 UTC-4	930 Compact...	Standard 6	Stand

Component name	Retention time [min]	Height [ $\mu\text{S}/\text{cm}$ ]	Area [ $(\mu\text{S}/\text{cm}) \times \text{min}$ ]	Concentration [ppm]
Fluoride	4.28	29.496	5.549	9.984
Chloride	6.02	89.534	17.220	48.984
Nitrite	7.02	19.217	4.698	19.789
Bromide	8.73	15.830	4.579	29.421
Nitrate	9.86	12.339	3.916	19.787
Phosphate	12.97	14.308	5.510	48.792

Settings	Peak detection	Events
Smoothing: 30		
Sensitivity: 50		
Basic setting		

Chromatogram: Anions. Chromatogram. 19.43 min. 116.39  $\mu\text{S}/\text{cm}$ . Peaks labeled: Fluoride 4.28, Chloride 6.02, Nitrite 7.02, Bromide 8.73, Nitrate 9.86, Phosphate 12.97, Sulfate 14.72.

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

Determination overview			
Filter	All determinations		
	Determination start ▼	Ident	
22	2018-06-21 15:54:00 UTC-4	IC Blank	
▶ 23	2018-04-11 14:27:26 UTC-4	Check Standard _R6	
24	2018-04-11 14:05:08 UTC-4	Check Standard _R5	
25	2018-04-11 14:42:50 UTC-4	Check Standard _R4	
26	2018-04-11 13:20:31 UTC-4	Check Standard _R3	
27	2018-04-11 12:58:13 UTC-4	Check Standard _R2	
28	2018-04-11 12:35:52 UTC-4	Check Standard _R1	
29	2018-04-11 12:13:26 UTC-4	Blank	
30	2018-04-10 21:16:13 UTC-4	Standard 6	
31	2018-04-10 20:53:52 UTC-4	Standard 5	
32	2018-04-10 20:31:32 UTC-4	Standard 4	
33	2018-04-10 20:09:11 UTC-4	Standard 3	
34	2018-04-10 19:46:50 UTC-4	Standard 2	
35	2018-04-10 19:24:30 UTC-4	Standard 1	
36	2018-04-10 19:02:10 UTC-4	Blank	

- Comment...
- Search...
- Filter ▶
- Batch ▶
- Sign ▶
- Show method...
- Show history
- Make current
- Detail overview...
- Overlay curves...
- Reprocess...**
- Complete

48

49

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

The screenshot displays the 'Reprocessing' software interface. At the top left is a 'Reprocessing table' with 8 rows of data. A callout '50' points to the first row. To the right is a 'Results' window showing a table of anions. Below these is the 'Evaluation parameters - Method from determination 1' window, which includes a 'Calibration curves' table and a 'Reprocess' dialog box. Callout '51' points to the 'Reprocessing' button at the bottom. Callout '52' points to the 'From selected determination' radio button in the 'Reprocess' dialog. Callout '53' points to the 'OK' button in the 'Reprocess' dialog. On the right side of the interface is a chromatogram showing peaks for various anions with their retention times labeled: Fluoride 4.28, Chloride 6.02, Nitrite 7.02, Bromide 8.73, Nitrate 9.86, Phosphate 12.87, and Sulfate 14.72.

Row	Start	Method	Ident	Sample typ
1	2018-04-11 12:13:26 UTC-4	930 Compact...	Standard 6	Standard 6
2	2018-04-11 12:13:26 UTC-4	930 Compact...	Blank	Sample
3	2018-04-11 12:35:52 UTC-4	930 Compact...	Check Stand...	Check stand
4	2018-04-11 12:58:13 UTC-4	930 Compact...	Check Stand...	Check stand
5	2018-04-11 13:20:31 UTC-4	930 Compact...	Check Stand...	Check stand
6	2018-04-11 13:42:50 UTC-4	930 Compact...	Check Stand...	Check stand
7	2018-04-11 14:05:08 UTC-4	930 Compact...	Check Stand...	Check stand
8	2018-04-11 14:27:26 UTC-4	930 Compact...	Check Stand...	Check stand

Component name	Retention time [min]	Height [µS/cm]	Area [(µS/cm) × min]	Concentration [ppm]
Fluoride	4.28	29.496	5.549	9.984
Chloride	6.02	89.534	17.220	48.984
Nitrite	7.02	19.217	4.698	19.789
Bromide	8.73	15.830	4.579	29.421
Nitrate	9.86	12.339	3.916	19.787

Component	Response	Curve type	Weight
1 Fluoride	Area	Quadratic	1/Concentration
2 Chloride	Area	Quadratic	1/Concentration
3 Nitrite	Area	Quadratic	1/Concentration
4 Bromide	Area	Quadratic	1/Concentration
5 Nitrate	Area	Quadratic	1/Concentration
6 Phosphate	Area	Quadratic	1/Concentration
7 Sulfate	Area	Quadratic	1/Concentration

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.