Metrohm-Peak

Ion Chromatography

MagIC Net Tutorial

Documents

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SECTION 1.0 IC SOLUTION PREPARATION

1.1 Eluent preparation

Making Eluent from Salts

1) Calculate the volume of desired eluent modifiers by their % composition in the eluent (if needed).

   Ex. Eluent with 15% acetone
   # ml acetone = volume of eluent x % modifier
   = 2000mL x 15% = 300mL acetone
   Will have 300mL of acetone in 1700 ml H_2O (2000mL – 300 ml).

2) Measure out desire quantity of ultrapure water (1 or 2L) in triple rinsed volumetric flask. Pour this into the triple-rinsed eluent bottle. Degas the water for 10-30 minutes while sonicating or stirring with a magnetic stirrer (degassing times may vary with the type of eluent modifier added). This removes micro-gas bubbles in the water.

3) Calculate the amount of salt needed to make the eluent:

   # g Salt = desired concentration **x** formula wt molarity **x** volume desired **x** (1/ percent composition for some salts/concentrates)

4) Zero a weighing boat on the analytical balance. Add the desired mass of salt. Record the actual mass.

5) Pour the salt into the eluent bottle containing the degassed ultrapure water (or wash it into the bottle with a portion of the Ultrapure water you degassed).

6) Thoroughly mix the solution by stirring with magnetic stir or sonication until salts are fully dissolved.

Making Eluent from a Concentrate

1) Proceed with step 1 as shown above, then use the formula below to calculate the amount of concentrate needed:

$$V_1 = \frac{C_2 \times V_2}{C_1} = \frac{\text{(Final Eluent Concentration)} \times \text{(Final Eluent Volume (ml))}}{\text{(Concentrated Eluent Concentration)}} = \text{Volume of Concentrate Needed (ml)}$$

2) Add this amount of concentrate to a volumetric flask of appropriate size, then dilute with ultrapure water to the desired volume. Carefully pour the eluent into the eluent bottle. Stir or sonicate while degassing the eluent for 5-20 minutes (degassing times may vary with eluent composition).

1.2 **Suppressor solutions** (for suppressed anion systems)

DI Water Rinse: Triple rinse 1L bottle marked UHP DI H_2O (rinse with ultrapure water). Fill bottle to approximately 1 L with ultrapure DI water.

100 mM H_2SO_4Regenerant: Triple rinse bottle with ultrapure water. Fill bottle to about 700 mL line with ultrapure DI water. Add 5.6 mL concentrated H_2SO_4 to the bottle. Fill the bottle to approximately 1L.

1.3 Calibration standards (Gravimetric standard preparation)

Make a Combined Stock Standard

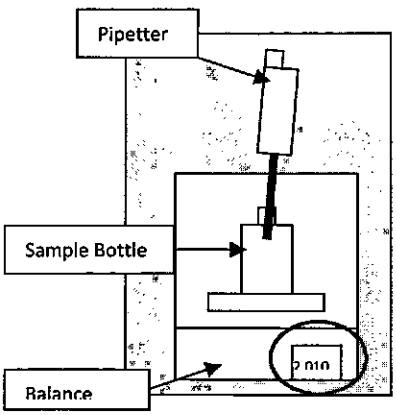
1. For a multipoint calibration it is easiest to first make a **Combined Stock Standard** from the 1000ppm individual ion concentrates. This stock can be used both as the highest calibration level, and be diluted to make the other standard levels. Make enough of this combined stock standard to use for the dilutions and to run on the IC (usually twice or more the amount of the other standards). Calculate the amount of **Individual Ion Concentrate** needed for each component ion in the **Combined Stock Standard**:

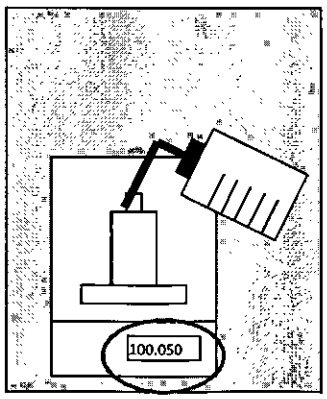
$$M_1 = \frac{C_2 \times M_2}{C_1} = \frac{\text{(Final Standard Concentration)} \times \text{(Final Standard Mass*)}}{\text{(Individual Concentrate Concentration)}} = \text{Initial Mass* of Individual Ion Concentrate Needed (g)}$$

Example: $M_1 = \frac{C_2 \times M_2}{C_1} = \frac{(20\text{ppm } SO_4^{2-}) \times (100\text{g})}{(1000\text{ppm } SO_4^{2-})} = 2$ g of 1000ppm SO_4^{2-} Concentrate Needed for 100mL of 20ppm standard

* Note: Because the specific gravity of water= 1g/ml, in these calculations you will be weighing out (in grams) the Initial Mass of Stock Standard Needed and Final Standard Mass rather than measuring out volume.

Be sure to use new pipette tip for each Individual Ion Concentrate to avoid cross-contamination of standards.





1. Place clean (preferably new) plastic bottle of appropriate size on the balance. Zero balance.
2. Add calculated **Initial Mass of Individual Ion Concentrate Needed** for a particular component ion to the bottle. Record the actual mass added to the limit of decimal places displayed by the balance. Repeat this procedure for each component ion, recording the actual mass of each ion added (do not zero balance in-between additions of component ions- keep a running total of mass). (Ex. 1.010 g of 1000ppm SO_4^{2-} added to 100mL bottle)
3. Add enough Ultrapure, IC grade water (16 MΩ or better) to bring the mass of solution up to the desired **Final Standard Mass**. Record the final mass achieved (to the limit of decimal places on the balance). Mark the appropriate concentration(s) on the standard bottle. (Ex. Standard diluted to 100.051 g)

4. Back calculate the actual concentrations of all ions in the Combined Stock Standard using this formula (or using an Excel Spreadsheet):

$$C_2 = \frac{C_1 \times M_1}{M_2} = \frac{\text{(Indv. Concentrate Concentration)} \times \text{(Stock Standard Added)}}{\text{(Final Standard Mass)}} = \text{Actual Ion Concentration in Stock}$$

Make Other Standard Levels by Serial Dilutions

5. Calculate the amount of **Combined Stock Standard** needed to make the other diluted standard levels:

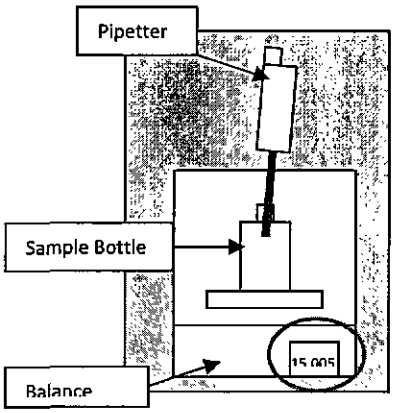
$$M_1 = \frac{C_2 \times M_2}{C_1} = \frac{\text{(Final Standard Concentration)} \times \text{(Final Standard Mass)}}{\text{(Stock Standard Concentration)}} = \text{Initial Mass of Stock Needed (g)}$$

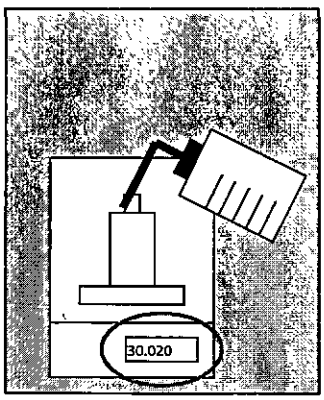
Ex. $M_1 = \frac{C_2 \times M_2}{C_1} = \frac{(10\text{ ppm}) \times (30\text{ g})}{(20\text{ ppm})} = 15$ g Combined Stock Standard Needed for 10ppm diluted standard (Level 4)

$M_1 = \frac{C_2 \times M_2}{C_1} = \frac{(5\text{ ppm}) \times (30\text{ g})}{(20\text{ppm})} = 7.5$ g Combined Stock Standard Needed for 5ppm Dil. Std. (Level 3)

$M_1 = \frac{C_2 \times M_2}{C_1} = \frac{(2.5\text{ ppm}) \times (30\text{ g})}{(20\text{ppm})} = 3.75$ g Combined Stock Standard Needed for2.5ppm Dil. Std. (Level 2)

$M_1 = \frac{C_2 \times M_2}{C_1} = \frac{(1\text{ ppm}) \times (30\text{ g})}{(20\text{ppm})} = 1.5$ g Combined Stock Standard Needed for1ppm Dil. Std. (Level 1)





6. Place clean (preferably new) plastic bottle of appropriate size on the balance (use smaller bottle- Ex. 30 mL). Zero balance.

7. Add calculated **Initial Mass of Stock Needed** for this standard level to the bottle. Record the actual mass added to the limit of decimal places displayed by the balance. This volume of stock contains all component ions desired in the appropriate ratios.

8. Now add enough Ultrapure, IC grade water (16 MΩ or better) to dilute the standard up to the appropriate Final Standard Mass, and record this mass. Label bottle with standard level. **Repeat this procedure for all standard levels.**

Standard Level	Amt. Stock Added (g)	Final Std. Mass (g)
4	15.005	30.020
3	7.510	30.040
2	3.752	30.056
1	1.511	30.005

Ex.

9. Back-calculate the actual concentration of each component ion in the stock and diluted standards using the following formula (or with the ***Standard Concentrations Calculator*** Excel Spreadsheet, which is much faster):

$$C_2 = \frac{C_1 \times M_1}{M_2} = \frac{\text{(Stock Standard Concentration)} \times \text{(Stock Standard Added)}}{\text{(Final Standard Mass)}} = \text{Actual Ion Concentration in Standard}$$

Ex.

Individual Ion Concentrations of Combined Stock Standard

Standard or sample	Ion	Concentration of Indiv. Ion Concentrate (C_1)		Mass added (M_1)		Total mass of standard (M_2)		Ion Concentration (C_2)
Stock	Chloride	(1000 ppm	X	2.025)	/	100.050	=	20.239 ppm
	Sulfate	(1000 ppm	X	2.010)	/	100.050	=	20.090 ppm

Individual Ion Concentration of Diluted Standard(s)

Standard or sample	Ion	Concentration of Combined Stock Std. (C_1)		Mass added (M_1)		Total mass of standard (M_2)		Ion Concentration (C_2)
L4	Chloride	(20.239 ppm	X	15.005 g)	/	30.020 g	=	10.116 ppm
	Sulfate	(20.090 ppm	X	15.005 g)	/	30.020 g	=	10.042 ppm
L3	Chloride	(20.239 ppm	X	7.510 g)	/	30.040 g	=	5.060 ppm
	Sulfate	(20.090 ppm	X	7.510 g)	/	30.040 g	=	5.022 ppm
L2	Chloride	(20.239 ppm	X	3.752 g)	/	30.056 g	=	2.526 ppm
	Sulfate	(20.090 ppm	X	3.752 g)	/	30.056 g	=	2.508 ppm
L1	Chloride	(20.239 ppm	X	1.511 g)	/	30.005 g	=	1.019 ppm
	Sulfate	(20.090 ppm	X	1.511 g)	/	30.005 g	=	1.012 ppm

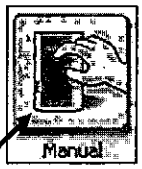
10. Run the standards on the IC.

SECTION 2.0 OPERATION

2.1 Purging the IC Pump

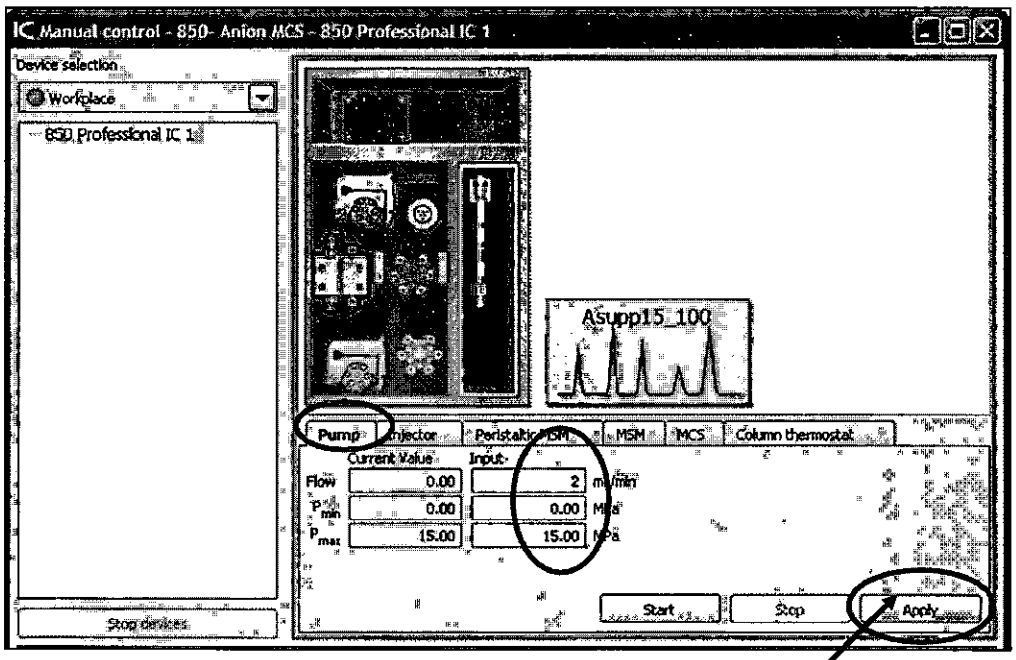
The IC pump should be purged when new eluent is put on the system, when air is observed in the lines and pressure is low, or when maintenance has been done on the IC pump.

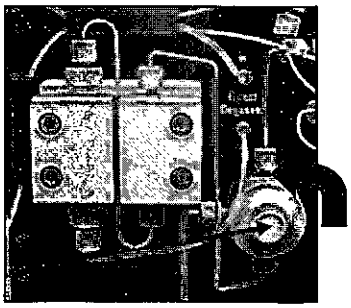
1. If the software is not already open, open it by double-left clicking on the MagIC Net 1.0 icon.



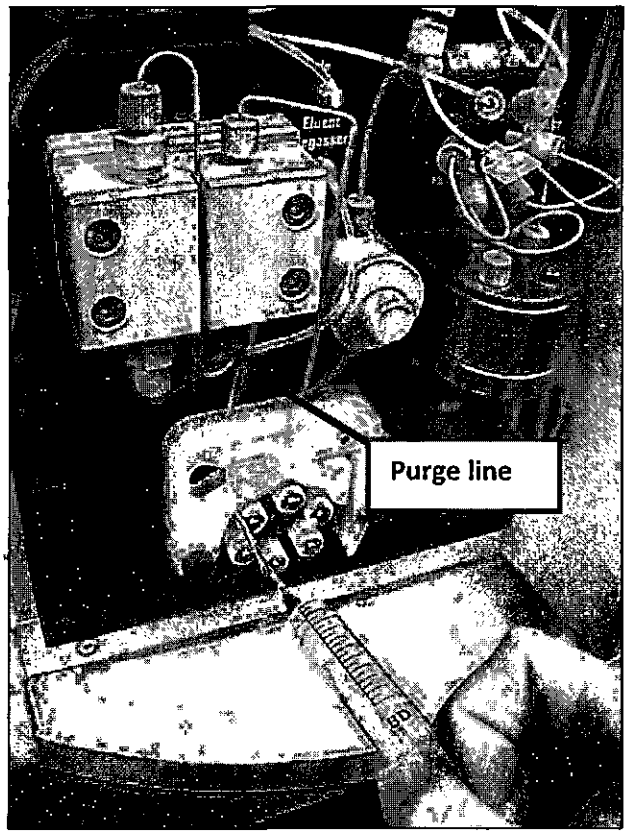
2. Click on the **Manual** icon at then bottom left of the MagIC Net screen. A Manual control window will open, displaying the components of the 850 IC.

3. Select the **Pump** tab (or click on the icon for the IC pump). Make sure the pump is shutdown (the **Stop** button is grayed-out). Change the **Flow Input** to **2 mL/min**. and the **P_{Min}** to **0.0 MPa**. Click the **Apply** button.





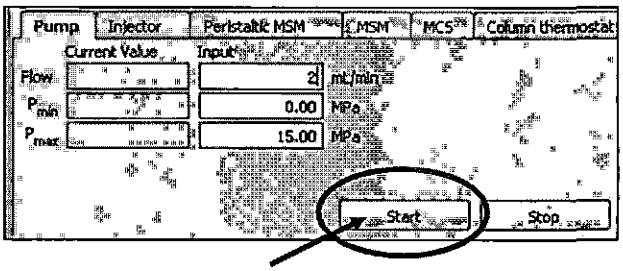
4. Open the door to the 850 IC, then turn the **purge valve knob <u>½ turn counter-clockwise</u>** to open it.



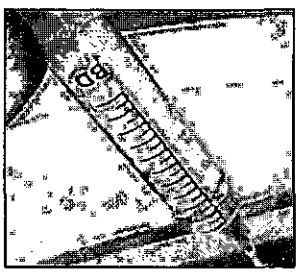
1. Connect a syringe with a Luer connection to the purge line of the IC pump.

2. Pull on the syringe with the purge valve open and the pump off until you see liquid beginning to enter the syringe. This purges air out of the eluent line and begins a gravity-fed eluent flow.

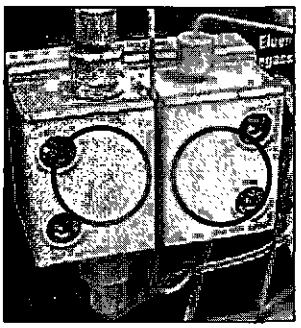
3. Turn on the IC pump by clicking the **Start** button in the Manual control window.



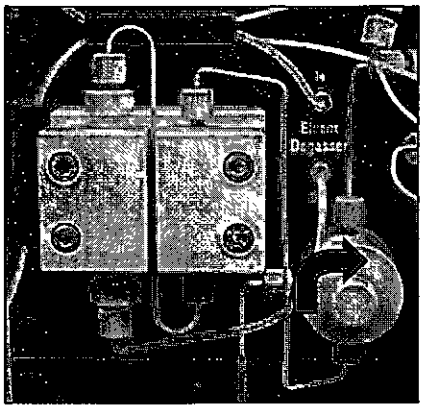
4. With the IC pump now running, pull the syringe plunger back to draw eluent into the syringe. Hold the pressure on the plunger until you can see that liquid is being steadily delivered into the syringe.



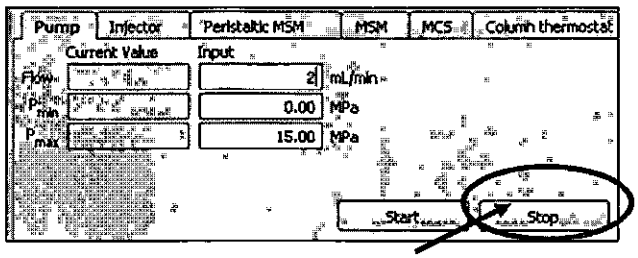
5. Release the pressure on the syringe plunger and allow it to equalize. Turn the syringe upside-down (plunger facing upwards, needle tip facing downwards). The liquid filling the syringe should be pushing the plunger outwards at an observable rate.



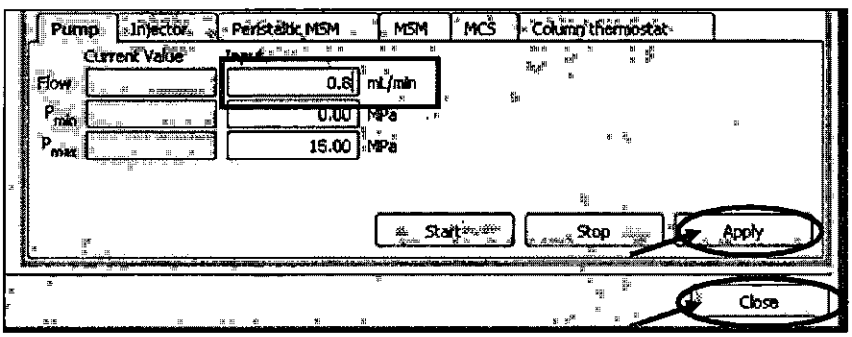
6. Tap the front of the pump head **lightly** on either side of division line while the pump is running. Observe whether or not air bubbles are passing into the syringe. If they do, continue lightly tapping the front of the pump head and the eluent line until air bubbles are no longer passing into the syringe.



7. Once fluid is observed flowing freely into the syringe and no air bubbles are observed, click **Stop** on the manual control window. Turn the purge valve knob clockwise until it is snug (finger-tight only).



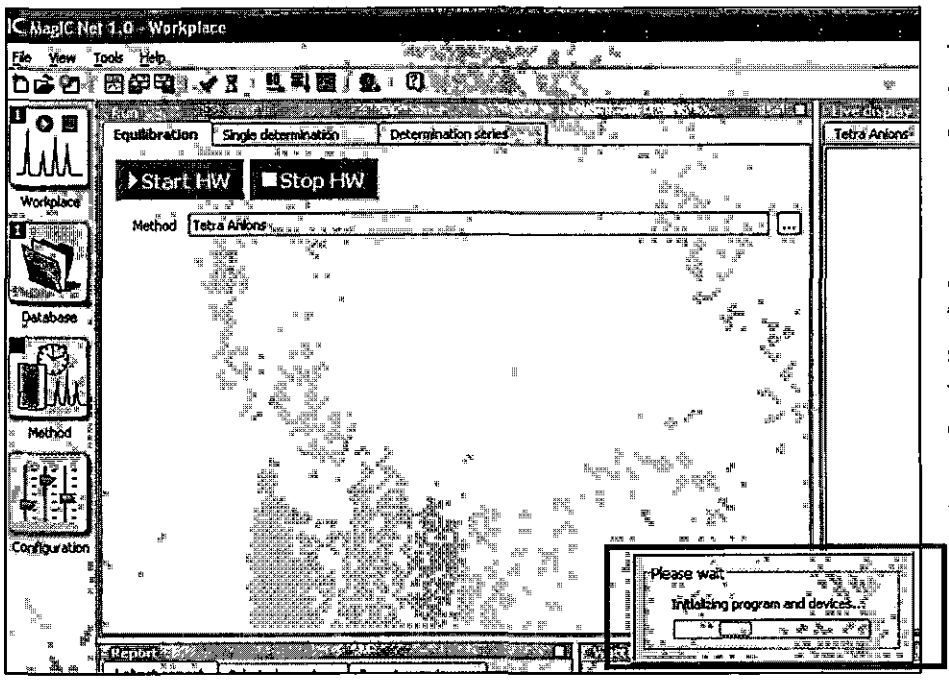
8. Change the **Flow input** back to the normal flow rate of the column (see column literature; E.g. 0.8 mL/min for Asupp 7 column). Click **Apply** and then **Close** the manual control window.



9. Purging is now complete and the system is ready to run.

2.2 System Startup

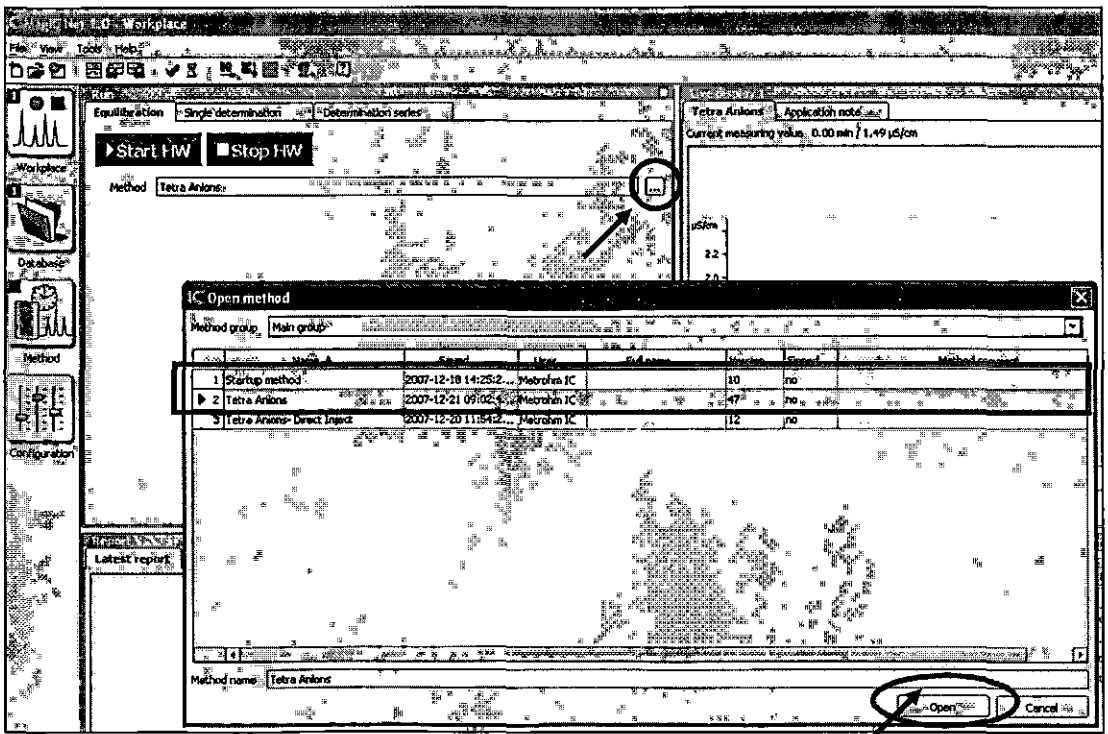
1. If the software is not already open, open it by double-left clicking on the MagIC Net 1.0 icon.



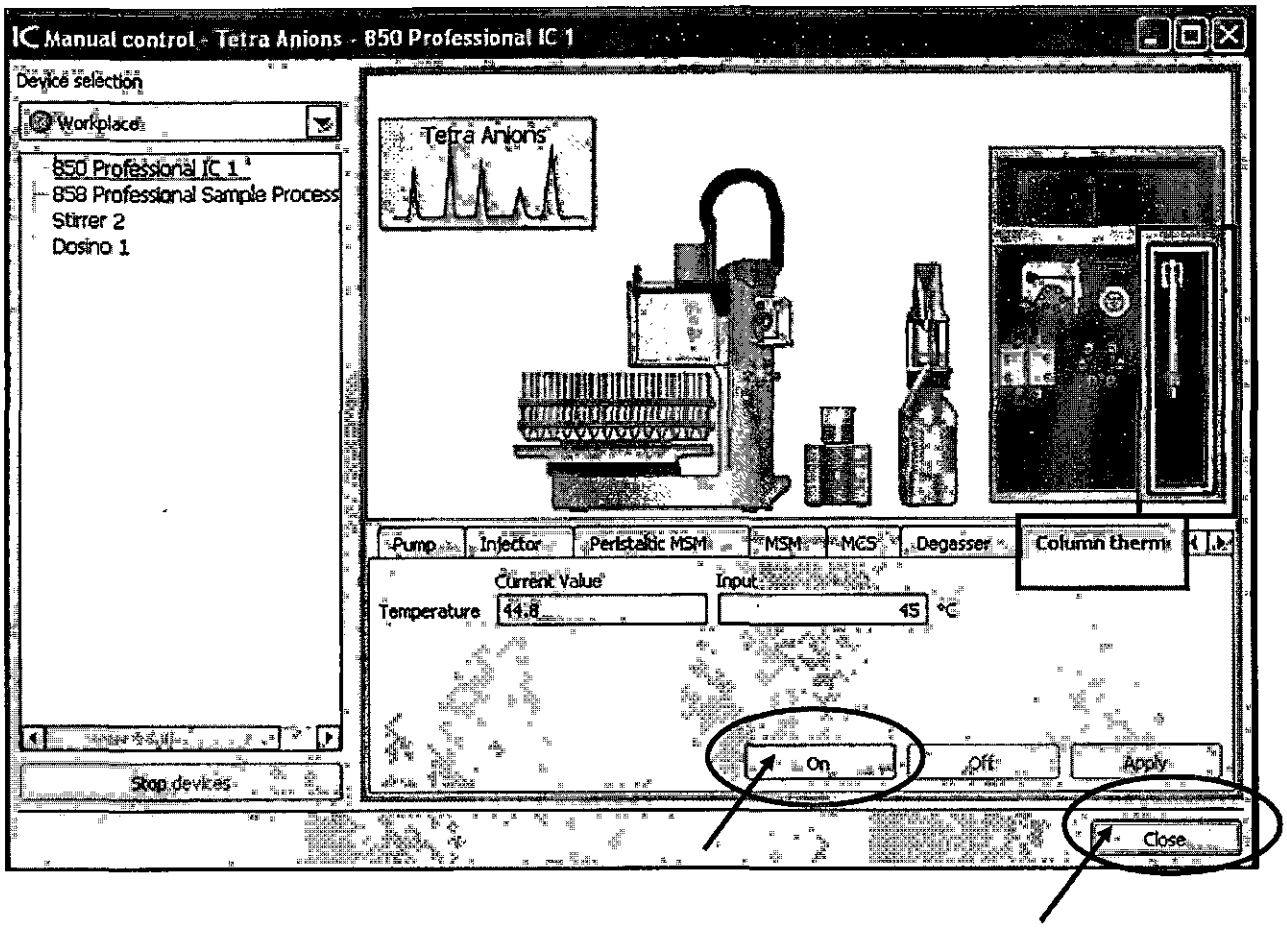
The main program window will open and will display a message indicating that the program and devices are being initialized. If an autosampler is connected to the system it will make several audible beeps and the needle and rack will go through an initialization process. If any devices designated in the method are not detected, a warning message to this effect will be displayed.

Startup Procedure

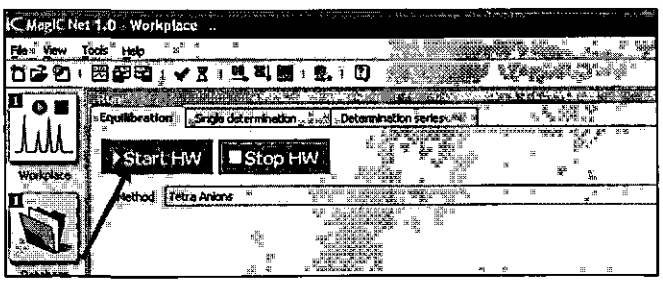
2. In the **Workplace** window, click on the  icon to select the method to be equilibrated (Ex. Tetra Anions). Then click **Open**.



3. Click the **Manual** button to open the **Manual control** window. In the picture of the 850 IC, click on the **Column thermostat** (alternately, use the arrows to scroll through the control windows to the **Column thermostat** tab). Click the **On** button to activate the column thermostat and begin bringing the column up to its proper temperature. You may then **Close** the **Manual control** window.

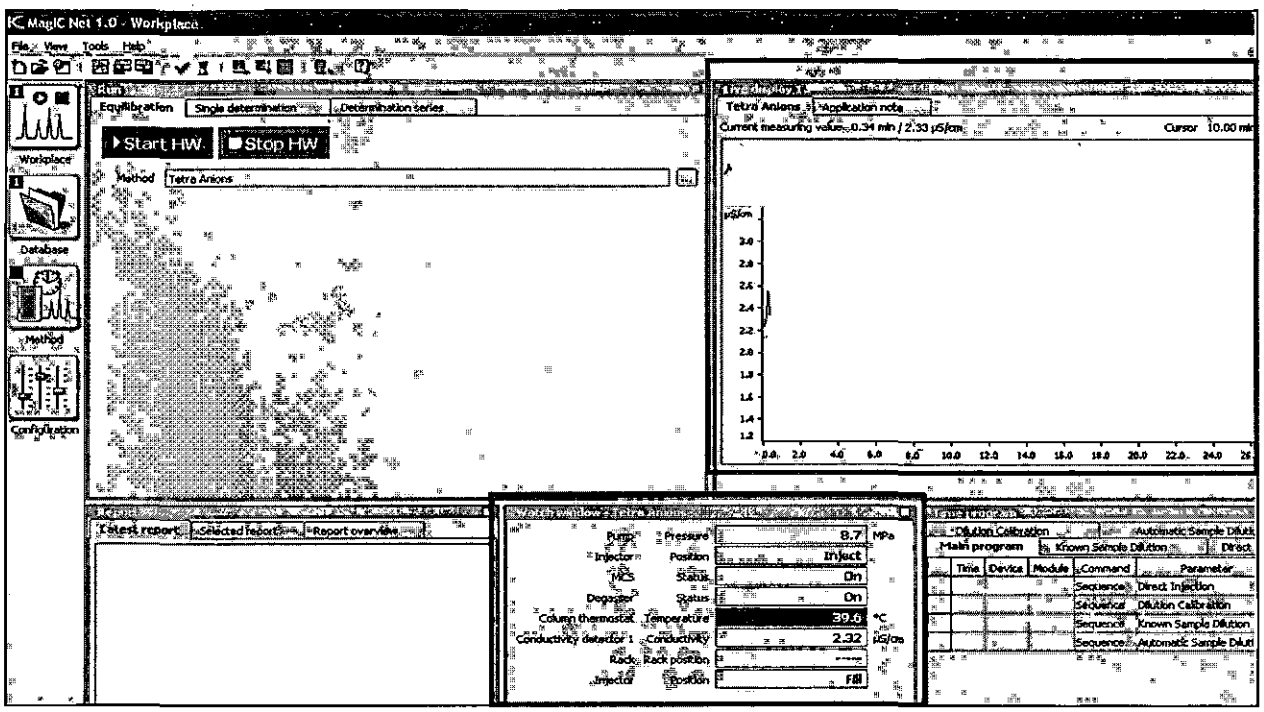


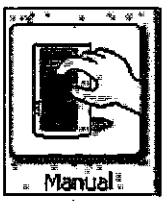
4. Allow the column thermostat to heat up for 5-10 minutes before starting up the equilibration of the column.



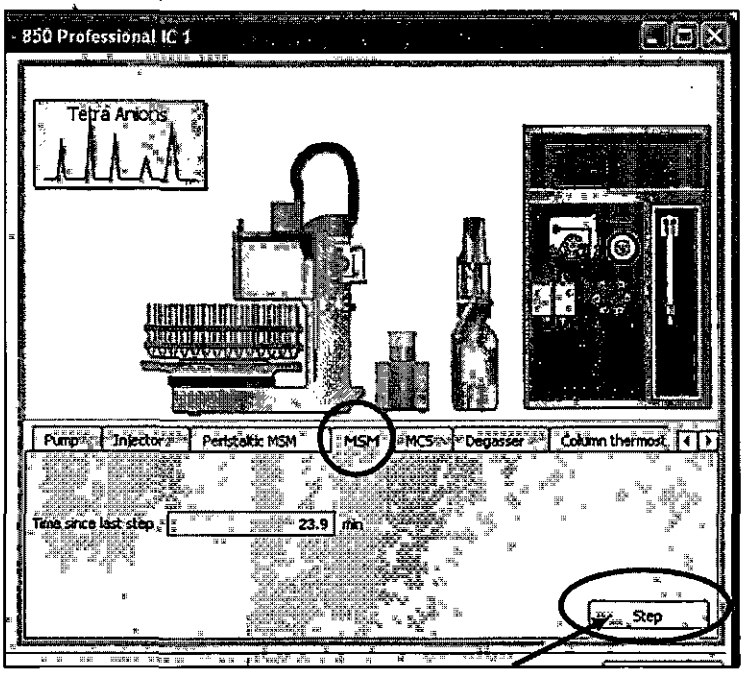
5. In the **Run** window of the **Workplace**, click on the **Start HW** button. This will begin the equilibration of the column.

6. A conductivity baseline will appear in the **Live display** window of the workplace, and the **Watch window** will display the current pump pressure, column themperature and conductivity reading.



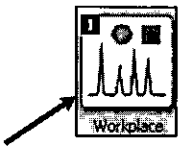


7. After the baseline has run for 10 minutes, click on the **Manual** control button. Select the **MSM** tab of the control window (Metrohm Suppression Module- this is the chemical suppressor).

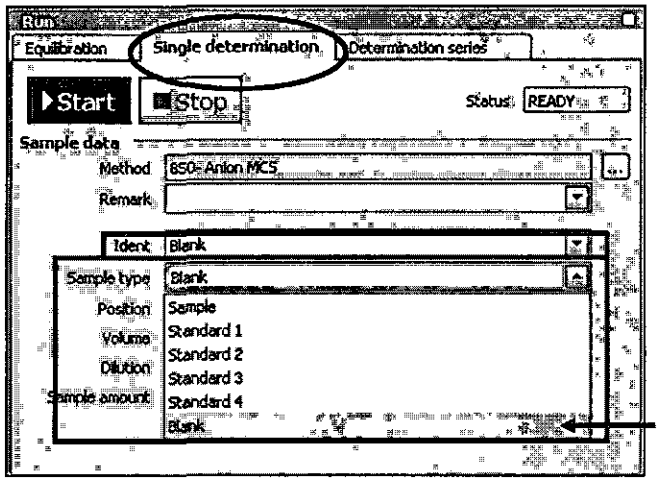


Click the **Step** button to rotate the suppressor to a new channel. The **Time since last step** window will reset. After 10 minutes has elapsed in this window, click the **Step** button again. This will be repeated once more after another 10 minutes has passed. This will allow all three channels of the suppressor to be regenerated prior to running samples. It is also a diagnostic step during the warm-up to determine the readiness of the suppressor.

2.3 Starting a Single Sample Determination



1. Click on the **Workplace** icon to the left of the MagIC Net screen.

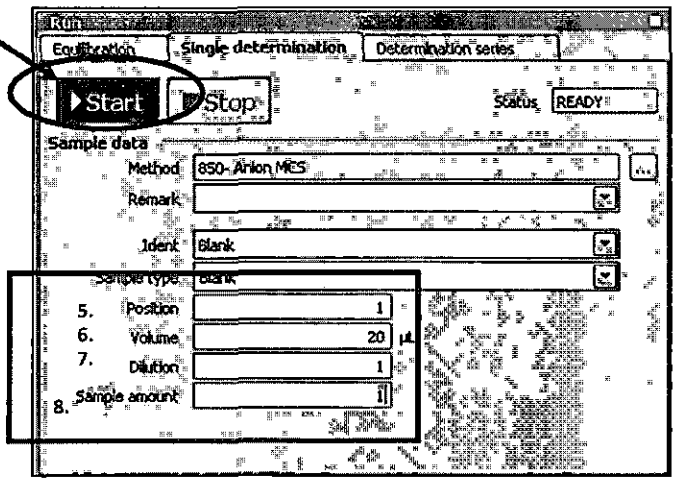


2. Select the **Single determination** tab in the **Run** window.

3. Enter sample identification in the **Ident** blank.

4. Select the **Sample type** from the pull-down menu (Ex. Blank)

9.



5. **Position**: The autosampler rack postion the sample is in; when not using an autosampler enter a "**1**" in this field.

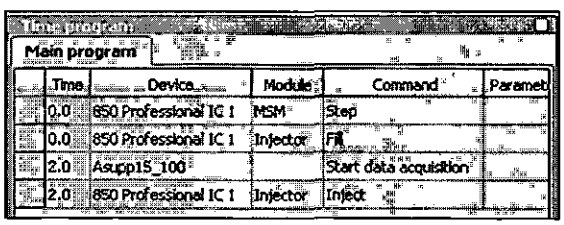
6. **Volume:** The sample loop size (Ex. 20 uL)

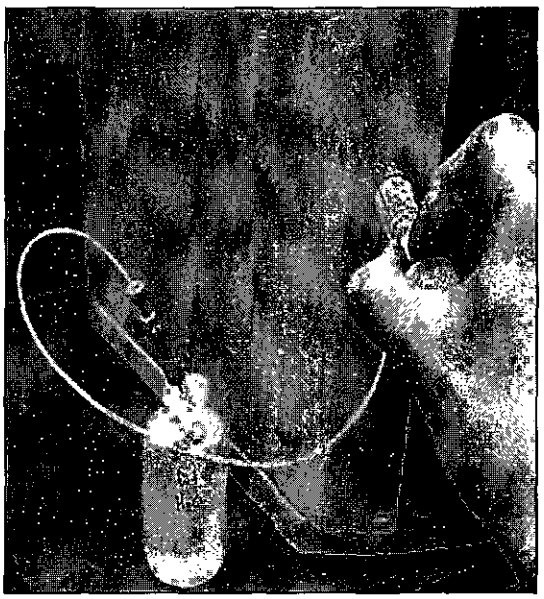
7. **Dilution factor**: The dilution factor of the sample; for example 100 would be entered for a 1:100 dilution. Enter a "1" for no dilution.

8. **Sample amount**: Enter a "1"; for automatic calculation of the dilution enter the amount of sample before dilution in this field and the final mass after dilution in the **Dilution factor** field.

9. Click **Start**

The time Program for the instrument will now begin.



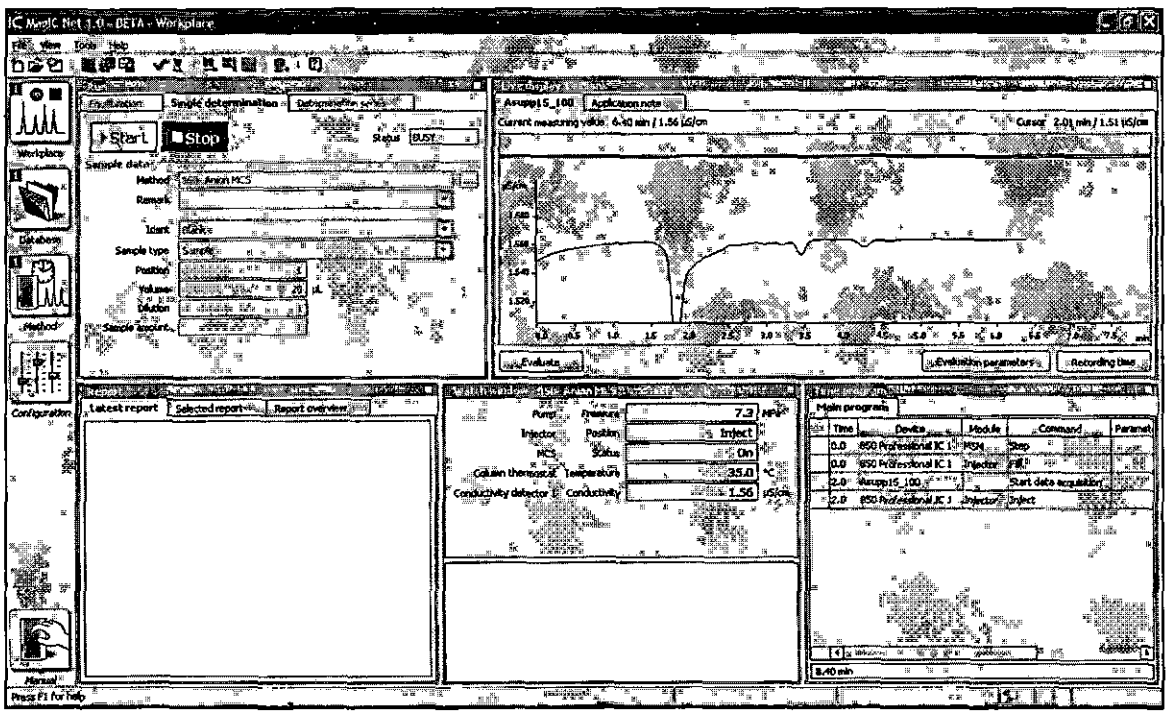


1. After you hear the sound of the valve switching, insert the sample line into the sample bottle and pull back on the syringe plunger to about the 2 mL marker.

2. Hold the syringe in this position until nearly 2 mL has been aspirated into the syringe. Slowly the release the plunger and allow the pressure in the syringe to equilibrate and the fluid to stop flowing.

3. Keep the sample line in the sample bottle until the valve goes into the inject position (and the baseline changes color and begins recording data). You may now remove the sample line from the bottle.

The chromatogram will now run for the allotted time.



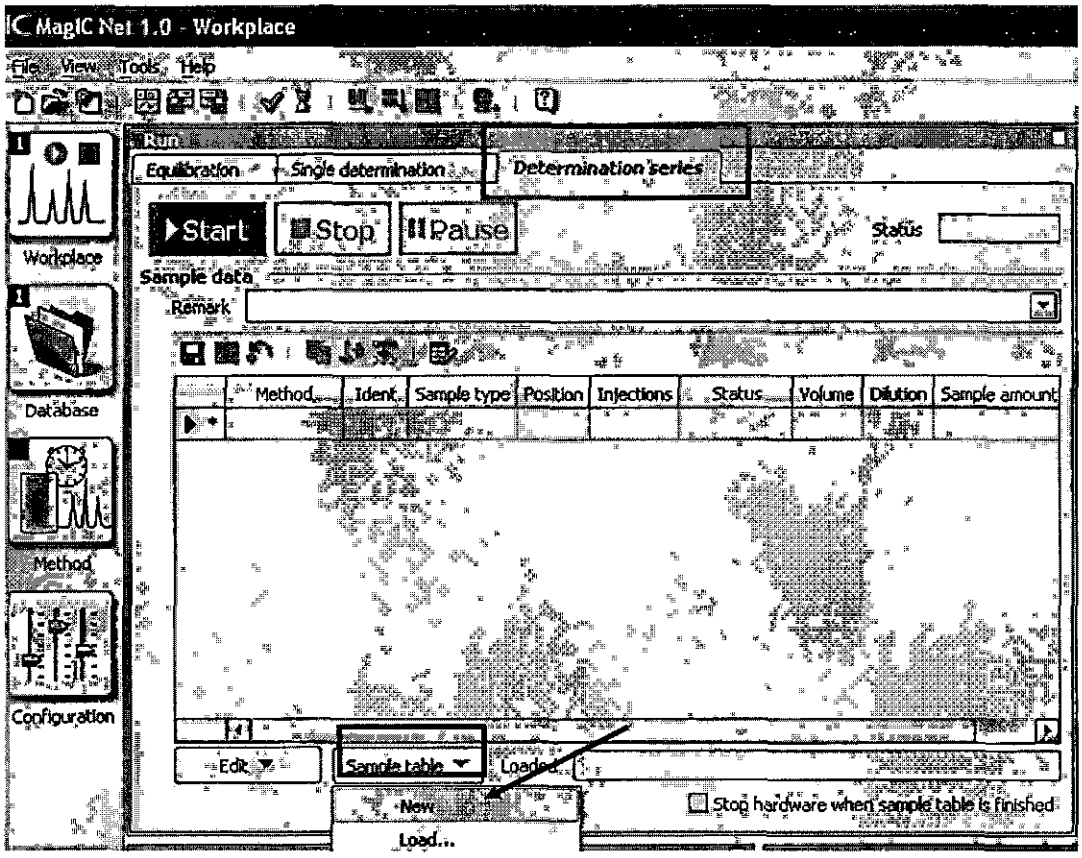
2.4 Starting a sample series

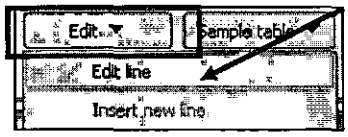
- The example that follows is a sample series for a calibration, consisting of the following: a blank, standards 1-5, and several samples. See the calibration section for advice on how often to calibrate the system.

- During daily operation when not calibrating, a common sample series might be: a blank (no dilution), a check standard (use level 2 standard, run with **Sample type=sample**), and all samples to be run (be sure to include appropriate dilution factors).

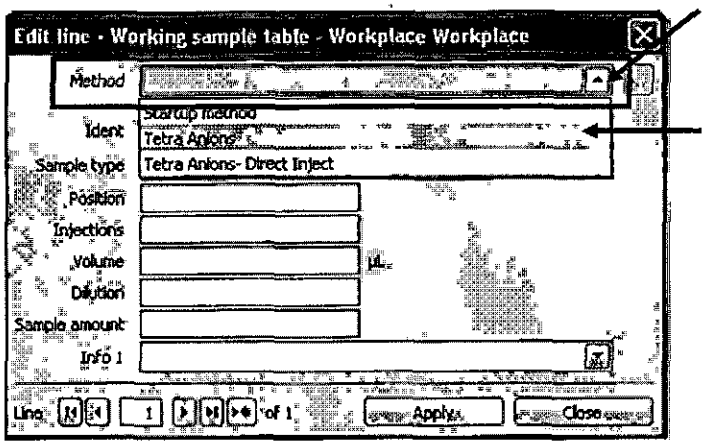
1. In the **Workplace** window, click on the **Determination series** tab.

2. Click on the **Sample table** button and select **New** to create a new sample table. To open an existing sample table select **Load** instead of **New** and then choose a sample table out of the selections given.

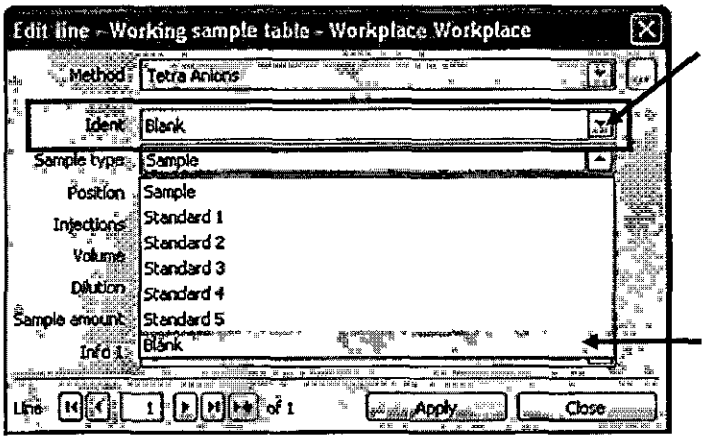




3. Add lines to a new sample table by clicking the **Edit** button, and then selecting **Edit line.**

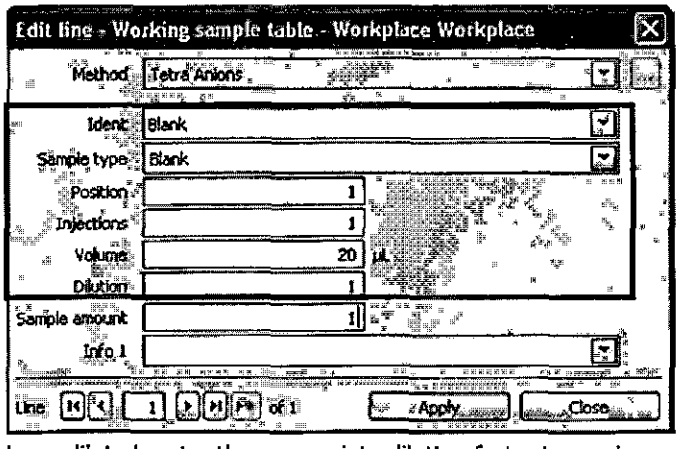


4. In the **Edit line** window that opens, use the pull-down menu to select the desired **Method** (Ex. Tetra Anions).



5. In the **Ident** field enter the desired sample or standard name.

6. In the **Sample type** filed use the pull-down menu to select the appropriate sample type. Only calibration standards should be labeled **Standard 1-5** (the level should increase as the concentration of the standard increases).



7. Enter the information for the following fields:

Position: The vial number on the autosampler rack

Injections: Number of injections made from the same vial (usually one)

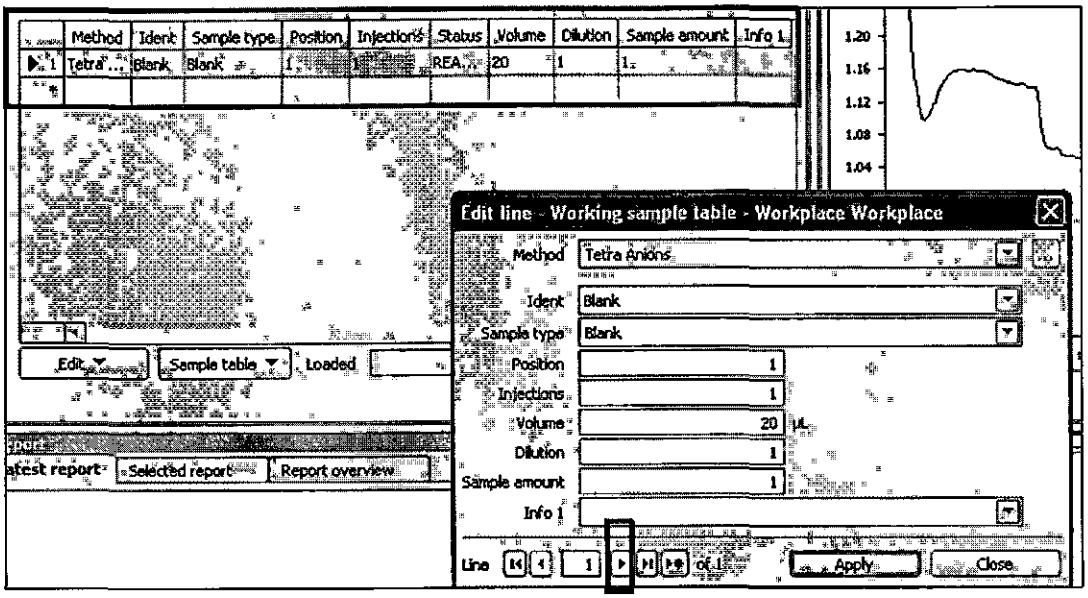
Volume (of the sample loop)

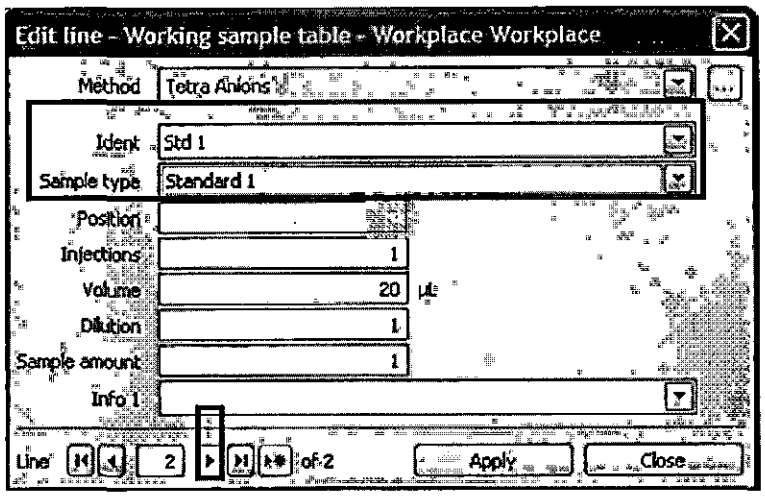
Dilution: The dilution factor of the sample- this should be 1 for blanks, undiluted samples, and standards made manually. For samples which have been diluted, enter the appropriate dilution factor to receive a calculation of the raw sample concentrations in the sample report (Ex. Enter "300" in this field for a 1:300 dilution). Note that systems with auto-dilution capability will actually dilute the sample or stock standard based on the number entered into this field.

Sample amount: This is a correction factor commonly used when dealing with samples of different density than the standard (see your application note for further details). When running standards made in water and sample diluted in water (the condition for most IC users), this value will be "1".

Info 1: Enter any special notes or comments you wish to make abut the sample.

8. Once you have entered the necessary information for a line, click the button on the **Edit line** window. The information will then appear in the sample table window and will increment the **Edit** line window to the next sample **Position.**





9. Enter the information for the following sample or standard:

Type in a new **Ident.** Use the pull-down to select the proper **Sample type**.

Vial **Position** has been incremented to the next vial (ex. Vial 2).

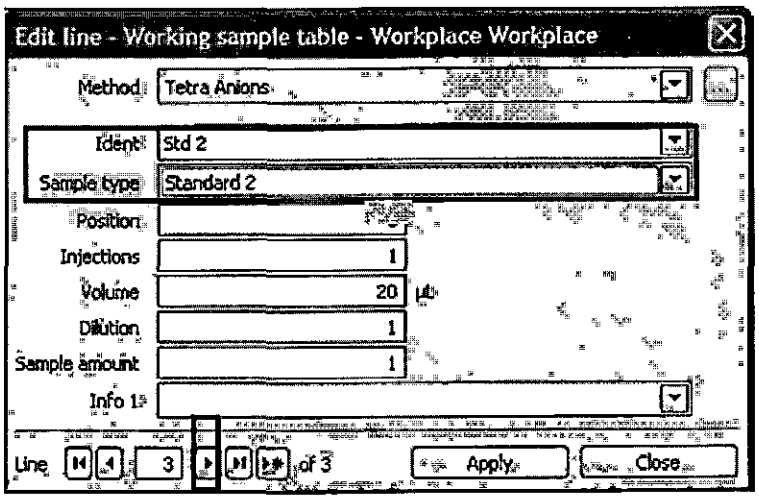
Injections should remain one unless a multiple injection series is being done (no more than two injections should be done from one vial).

Volume should not change.

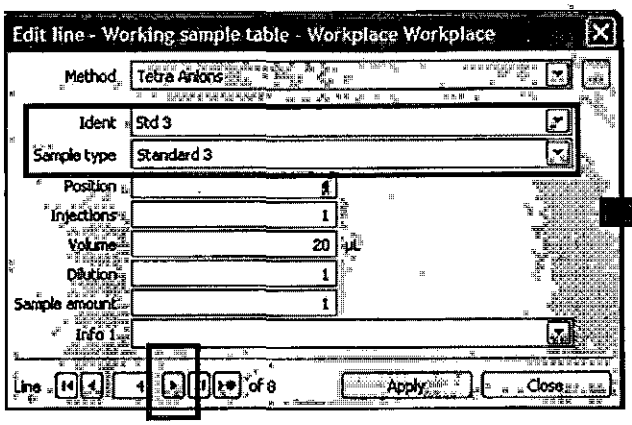
Dilution should be "**1**" for manually diluted standards or samples and blanks. Add the appropriate dilution factor for calibration standards being made automatically from a concentrated stock, or samples being automatically diluted.

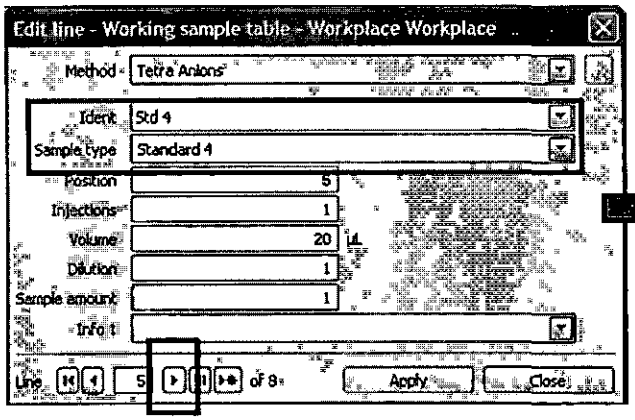
Sample amount should remain "**1**".

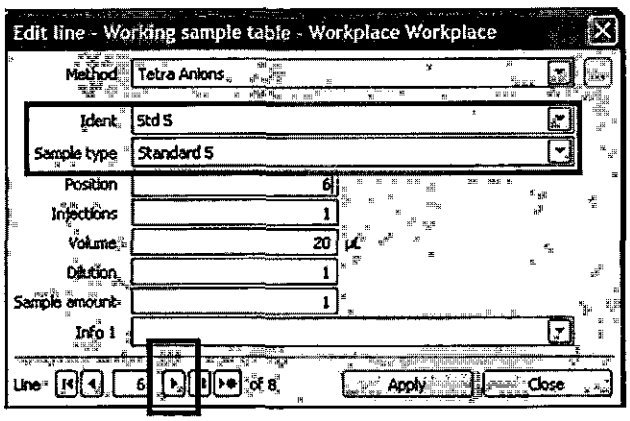
Click the button on the **Edit line** window to apply this information to the sample table and to increment to the next vial position.

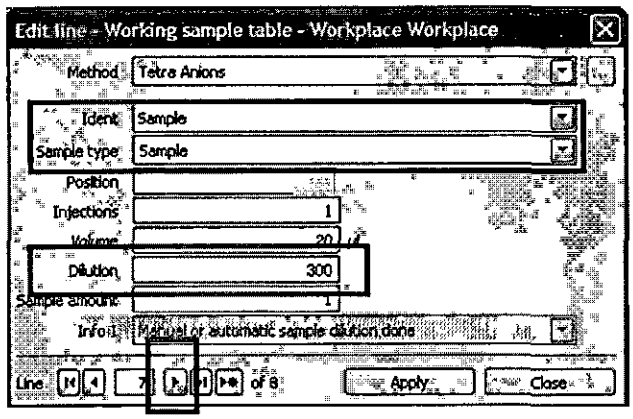


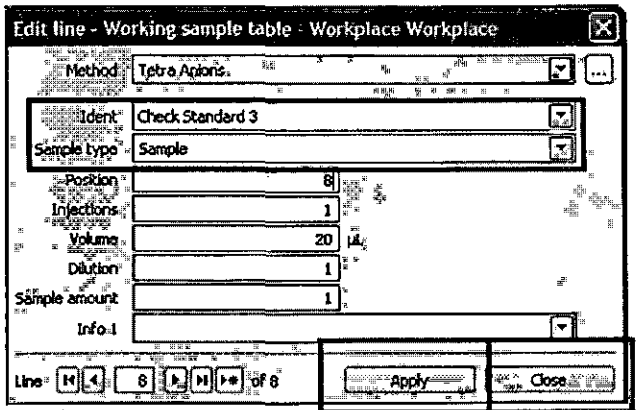
Select the next Standard number from the **Sample type** window. Click ▶ when all sample information has been changed to apply the information for this line and increment to the next line of the sample table. Click **Apply** to fill in the last line of the sample table. Click **Close** once all lines of the sample table have been added and applied.



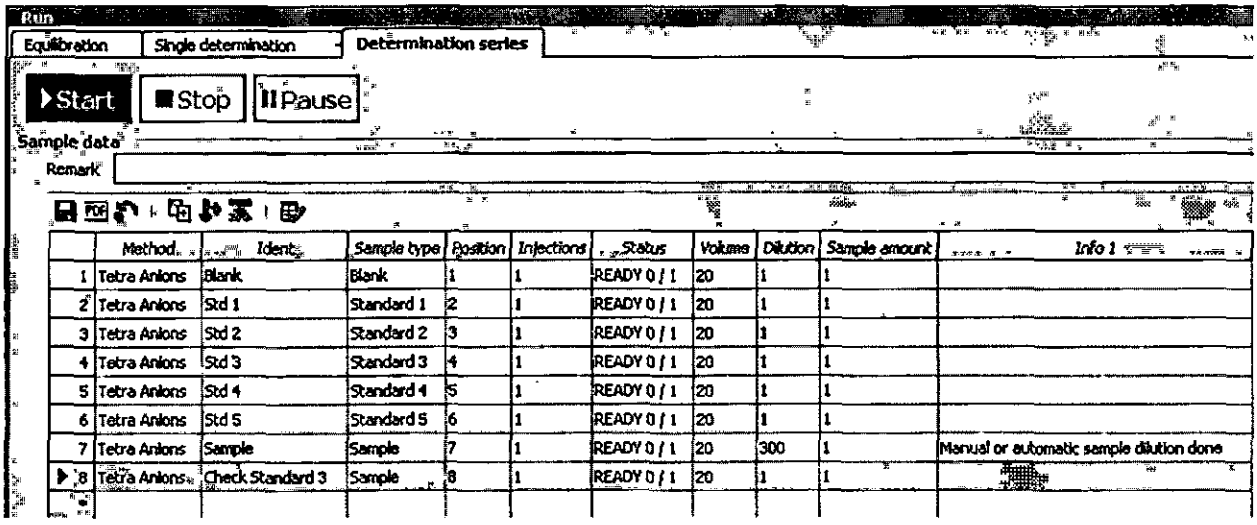




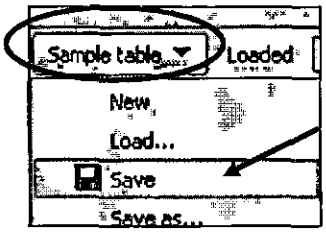




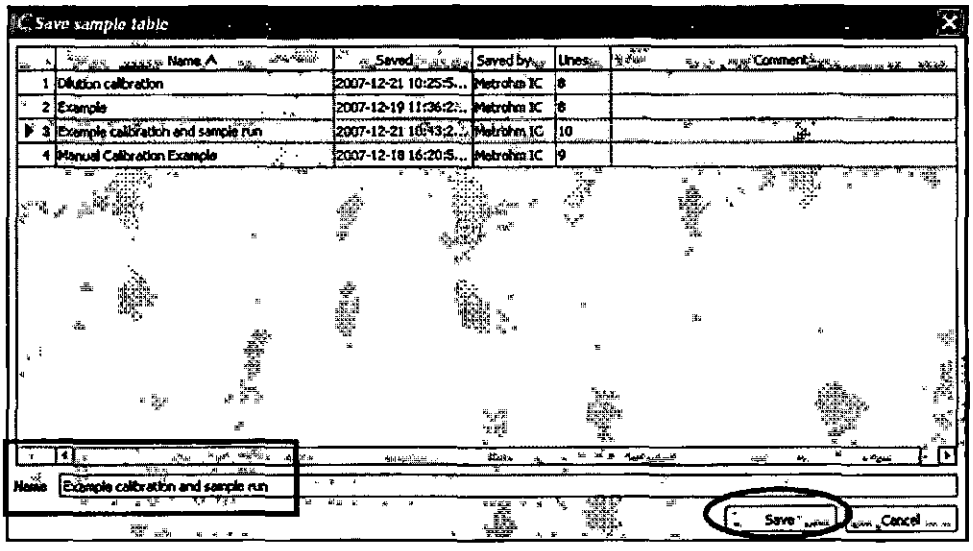
For the last line of the sample series, **do not** click ▶, **but rather** click **Apply**, then **Close.** Be sure that check standards are entered with a dilution factor of "**1**" and have a **Sample type** of "**Sample**". To avoid calculation errors, be sure to enter the proper dilution factor for samples run. **A completed sample table is shown on the following page.**



	Method	Ident	Sample type	Position	Injections	Status	Volume	Dilution	Sample amount	Info 1
1	Tetra Anions	Blank	Blank	1	1	READY 0 / 1	20	1	1	
2	Tetra Anions	Std 1	Standard 1	2	1	READY 0 / 1	20	1	1	
3	Tetra Anions	Std 2	Standard 2	3	1	READY 0 / 1	20	1	1	
4	Tetra Anions	Std 3	Standard 3	4	1	READY 0 / 1	20	1	1	
5	Tetra Anions	Std 4	Standard 4	5	1	READY 0 / 1	20	1	1	
6	Tetra Anions	Std 5	Standard 5	6	1	READY 0 / 1	20	1	1	
7	Tetra Anions	Sample	Sample	7	1	READY 0 / 1	20	300	1	Manual or automatic sample dilution done
8	Tetra Anions	Check Standard 3	Sample	8	1	READY 0 / 1	20	1	1	



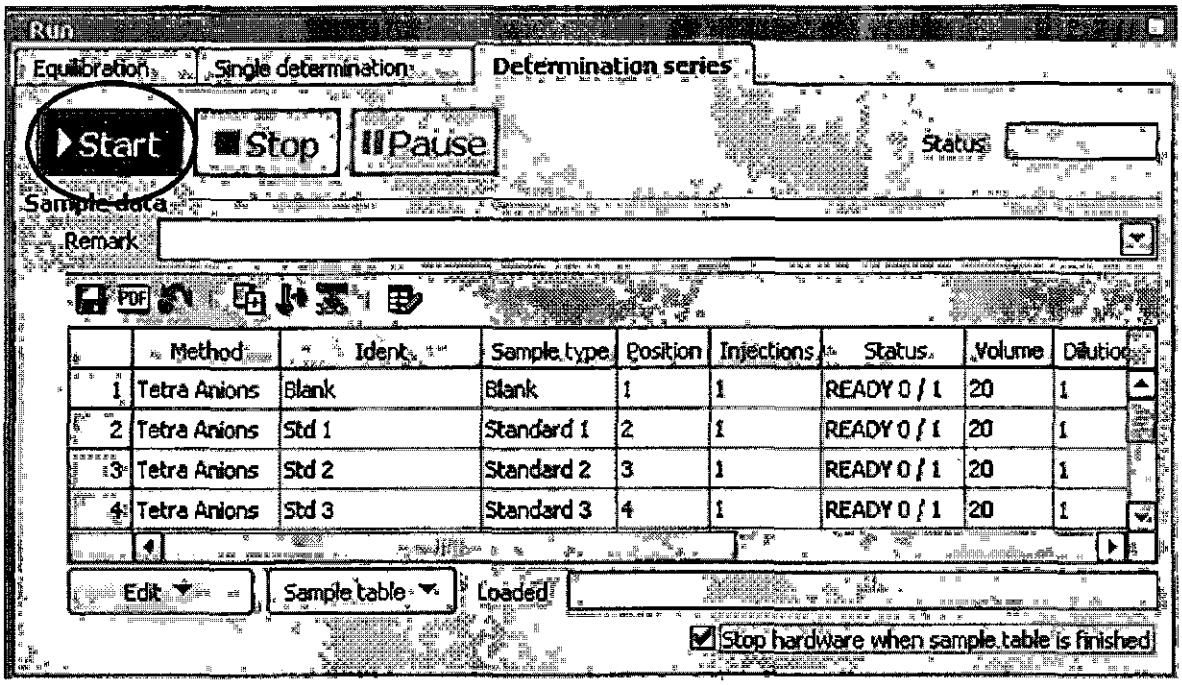
10. To save a completed sample table click the **Sample table button** and then select **Save**. Name the sample table appropriately in the **Save sample table** window that comes up, and click the **Save** button.



Enter the appropriate name for the sample table. Click **Save** when done.

11. If you want the instrument to shutdown after finishing all the lines of the sample series, click the **Stop hardware when sample table is finished** checkbox.

12. To start the sample series click the green **Start** button.



2.5 Calibration

Frequency of calibration: Some laboratories operate under regulations requiring recalibration with every sample series that is run (a full set of standards is run before any samples are run in the series), and some laboratories are able to operate with less frequent calibration (recalibrate only when major changes are made to the system or when a check standard falls outside of 5-10% of the expected value). Here are some general guidelines for when recalibration is recommended:

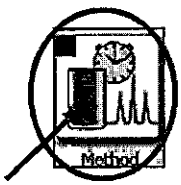
1) When new eluent is made (slight changes in eluent concentration from batch to batch can cause slight shifting of peak retention times and potential mislabeling of peaks).

2) When a major change is made to the system (PM maintenance is done on the IC pump, a new column or guard column is put on, or autosampler peristaltic pump tubing is changed).

3) When a check standard (usually from the low-mid end of the calibration range) that is run as a sample falls outside 5-10% of the expected concentration value.

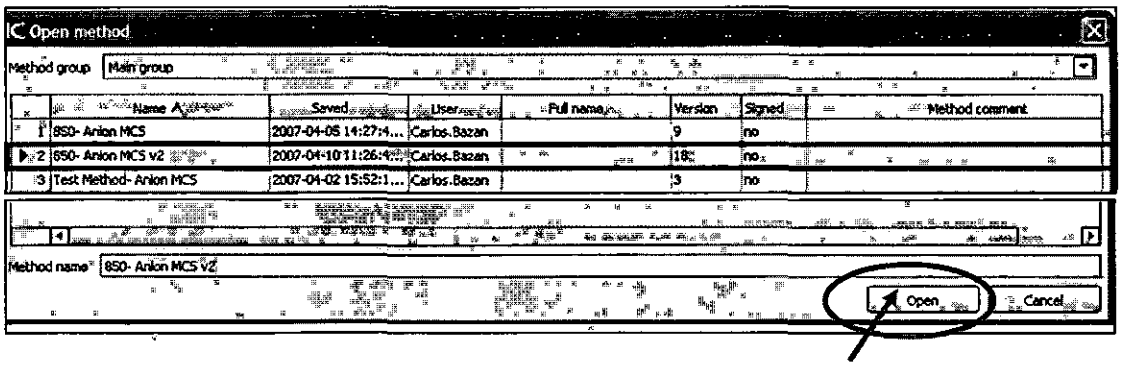
4) When new analyte ions are added to the analysis.

I. INITIAL CALIBRATION OF A METHOD (for first use of a system or a method)

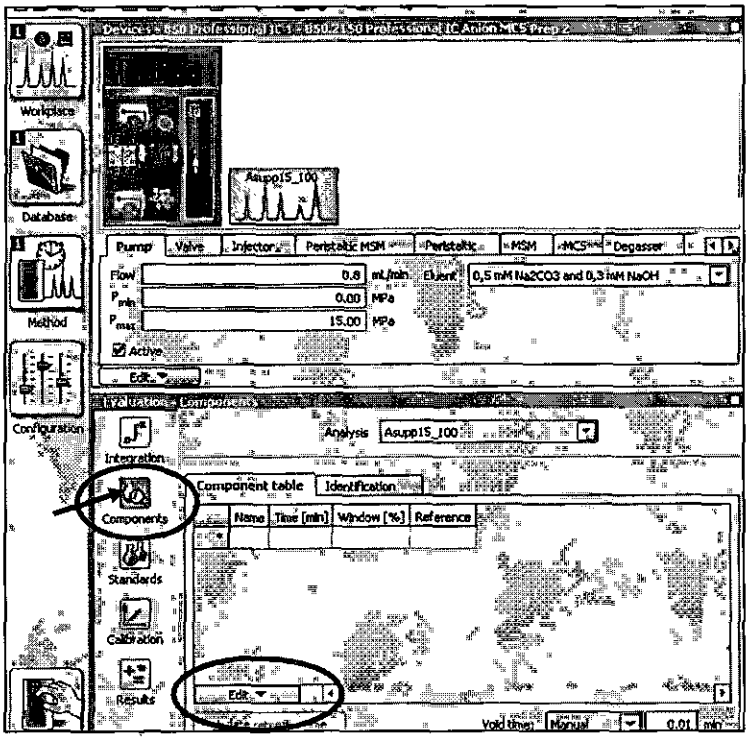


1. To begin a calibration, click on the **Method** icon to the left of the MagIC Net screen.

2. Open the Method to be used in calibration by going to **File > Open**, select the Method (e.g. 850- Anions MCS v2), and click **Open**.

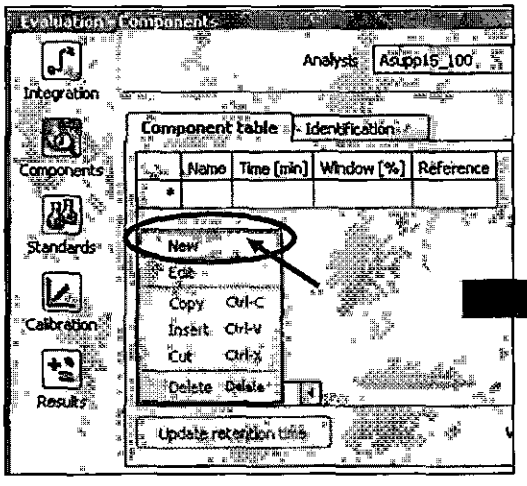


Edit Components

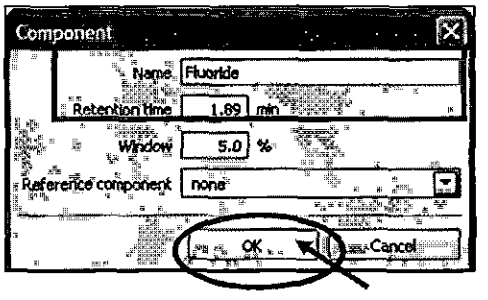


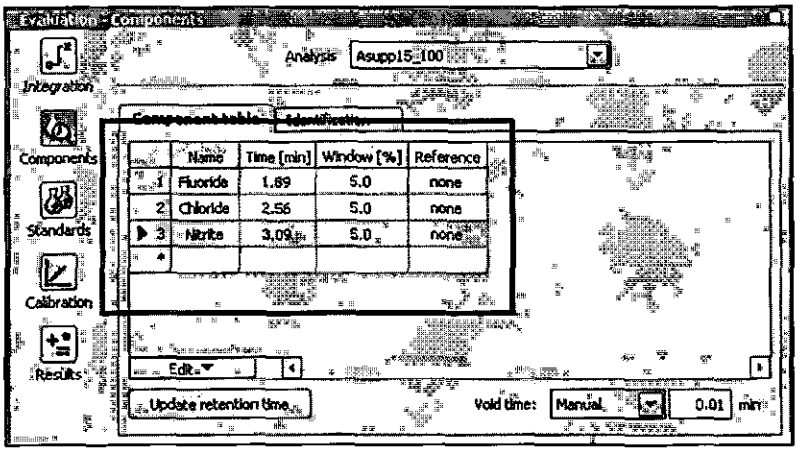
3. In the Evaluation window click on the **Components** icon.

4. Press the **Edit** button.



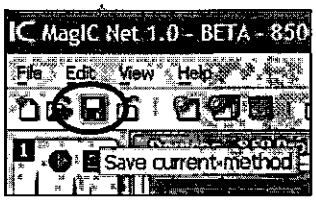
5. Select **New**. In the **Component** window that opens, enter the **Name** of the component and its **retention time** as seen in the column literature. Click **OK**.



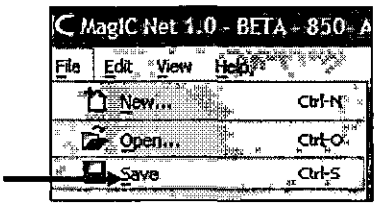


6. Repeat step 5 for each ion in the standard.

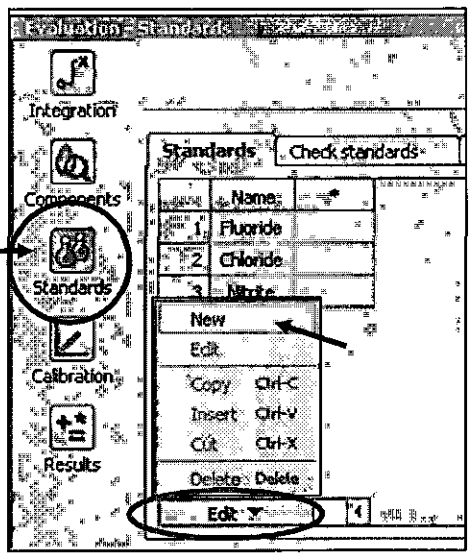
7. Save the changes to the Method by clicking the **Save current method** icon, or by going to **File > Save.**



or

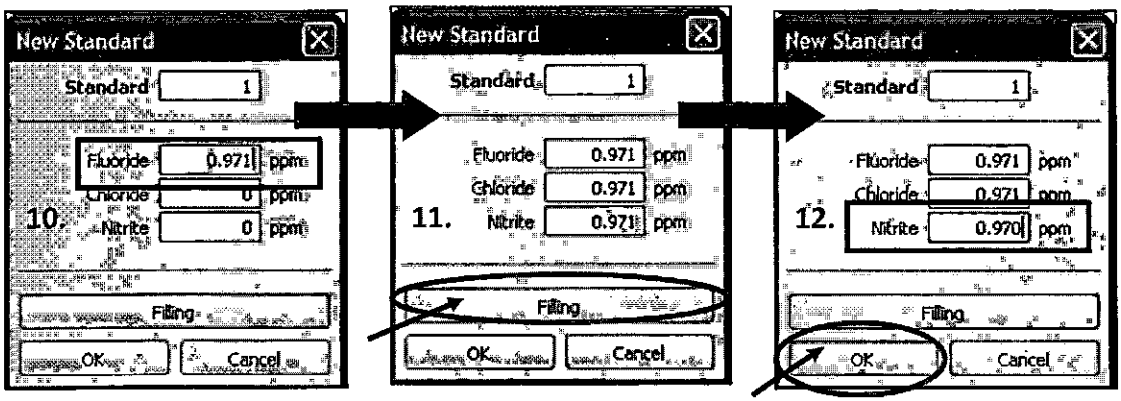


Enter standard concentrations



8. To enter standard concentrations, click on the **Standards** button in the **Evaluation** window of the **Method.**

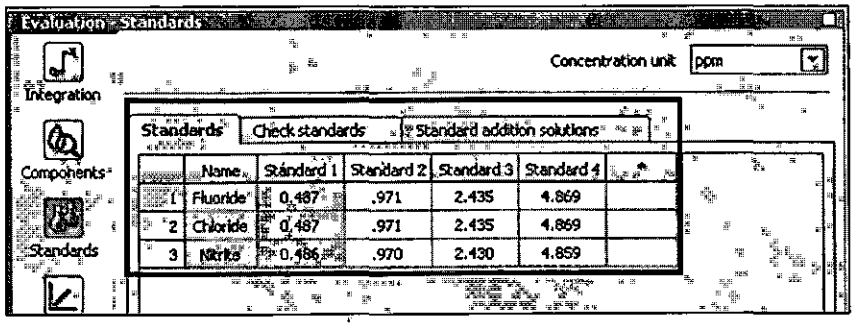
9. Left click on the **Edit** button, and then select **New.**



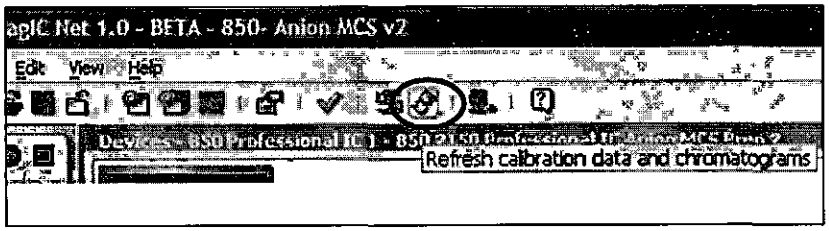
10. Enter the concentration for the first component in Standard 1.

11. If all the other analyte concentrations are the same or similar, click **Filling** to copy the highlighted concentration into all other cells.

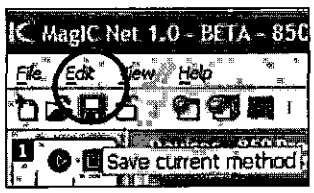
12. Make any minor changes necessary to the concentrations and click **OK.**



13. Repeat steps 9-12 for each standard level (Ex. Standards 1-4).



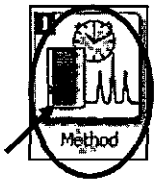
14. You should now refresh the calibration data by clicking on the **Refresh** button .



15. Save the Method by clicking on the **Save current method icon,** .

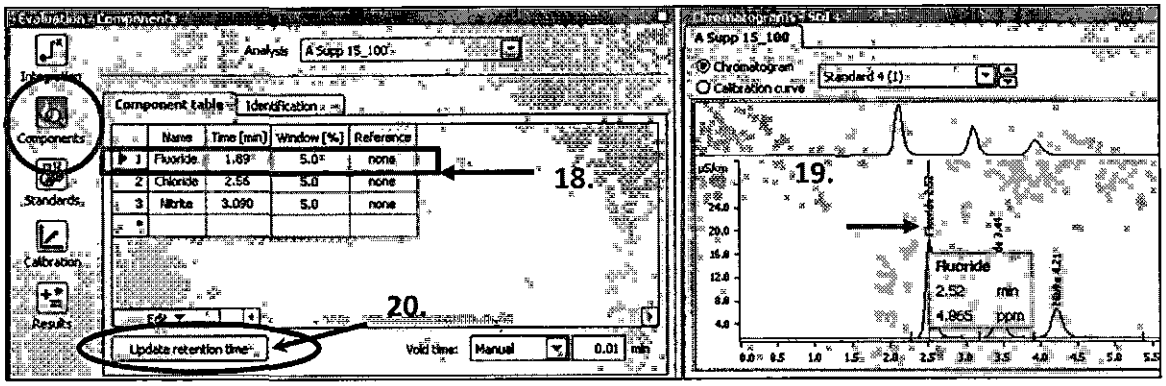
16. Run all calibration standards according to the instructions found in **Section 2.3 Starting a Single Sample Determination** or in **Section 2.4 Starting a Sample Series.**

Update retention times



17. Once the calibration curves have been run, move to the **Method** window again by clicking on the **Method** button on the left.

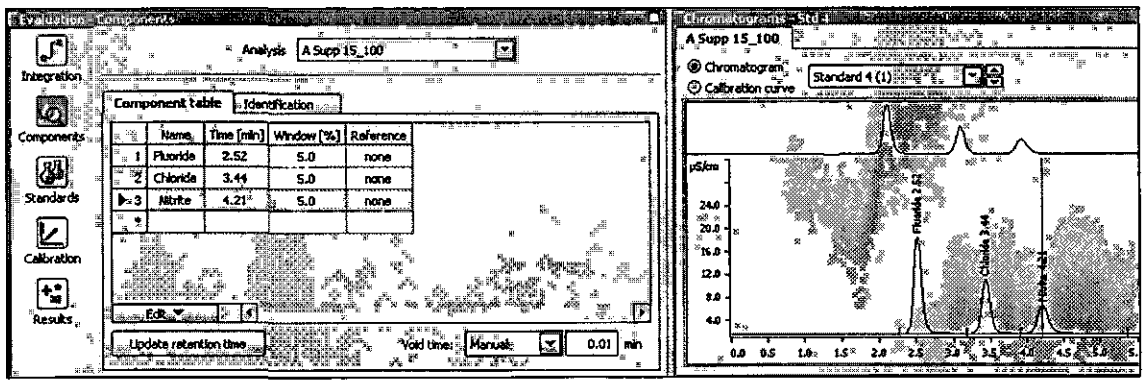
18. Click on the **Components** button in the **Evaluation- Components** window of the method. Then left click on the line of the component table for the first analyte ion (Ex. Fluoride). This line of the component table will become highlighted in yellow.



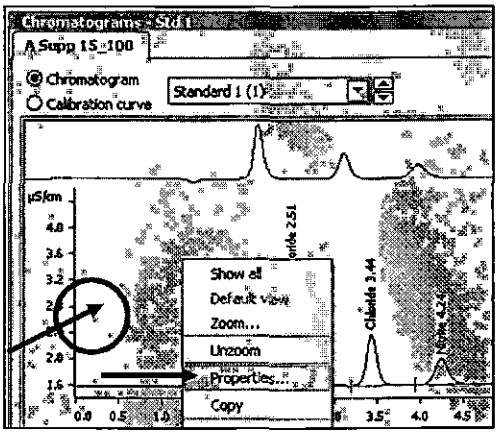
19. Now left click on the first peak of the **Chromatogram**; the peak will become highlighted in blue with the Retention time displayed in a pop-up box.

20. Once the first peak is highlighted, click the **Update retention time** button to update the stored retention time in the component table with the new retention time from the chromatogram on the left.

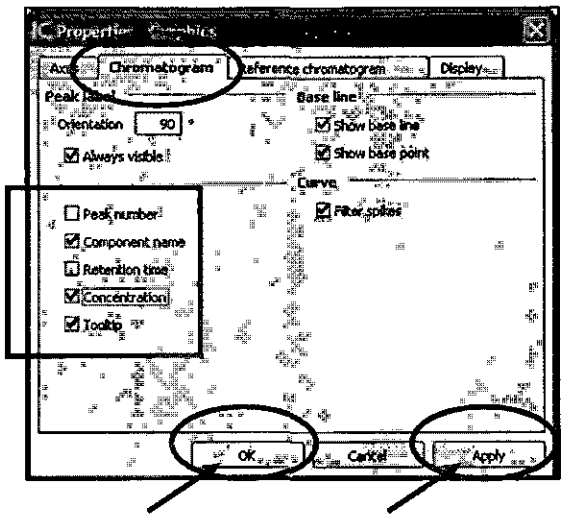
21. Repeat steps 18-20, clicking on each peak of the chromatogram and updating the retention time appropriately.



Edit chromatogram labeling



22. In the **Chromatogram** window of the Method, right click on the background of the window. Select **Properties** in the pop-up menu that appears.



23. In the **Graphics** window that arises, click on the **Chromatogram** tab.

24. Select the desired chromatogram peak labels. Multiple items may be selected (Ex. **Component name** and **Concentration**).

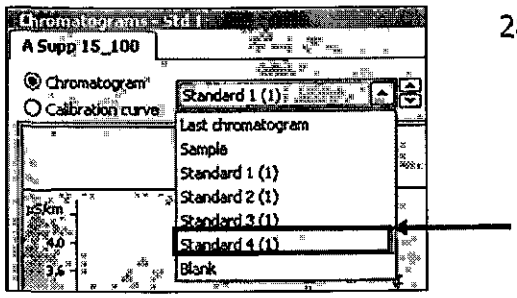
25. Click **Apply** and **OK.**

26. You should now refresh the calibration data by clicking on the **Refresh** button .

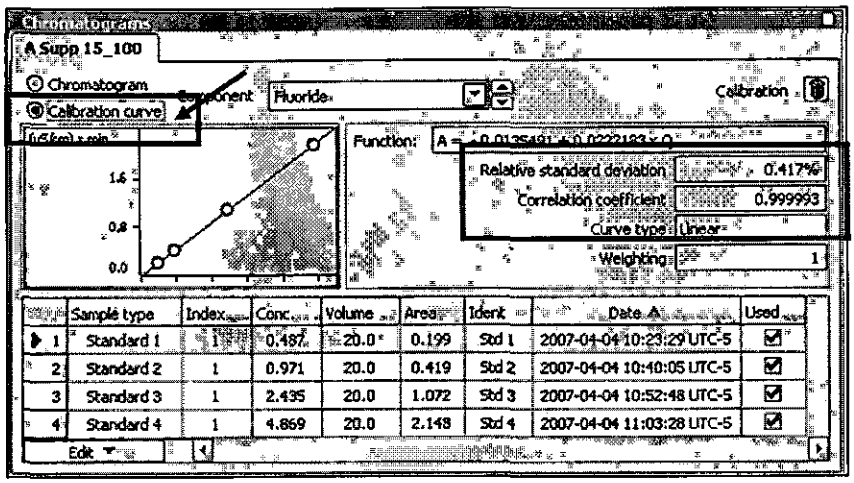
27. Save the Method by clicking on the **Save current method icon** .

The calibration is now complete.

Evaluate the calibration graph

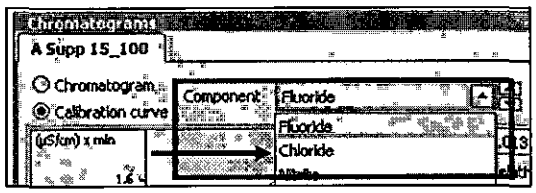


28. Use the pull-down menu on the chromatogram window of the method to select the last standard run (Ex. Standard 4).



29. Click on **Calibration curve.**

A good calibration curve will have a **Relative standard deviation** of 5% or less and a **Correlation coefficient** of 0.999.



30. Use the Component pull-down menu to scroll through the calibration graphs for the other component ions. Check their Relative standard deviation and correlation coefficients also.

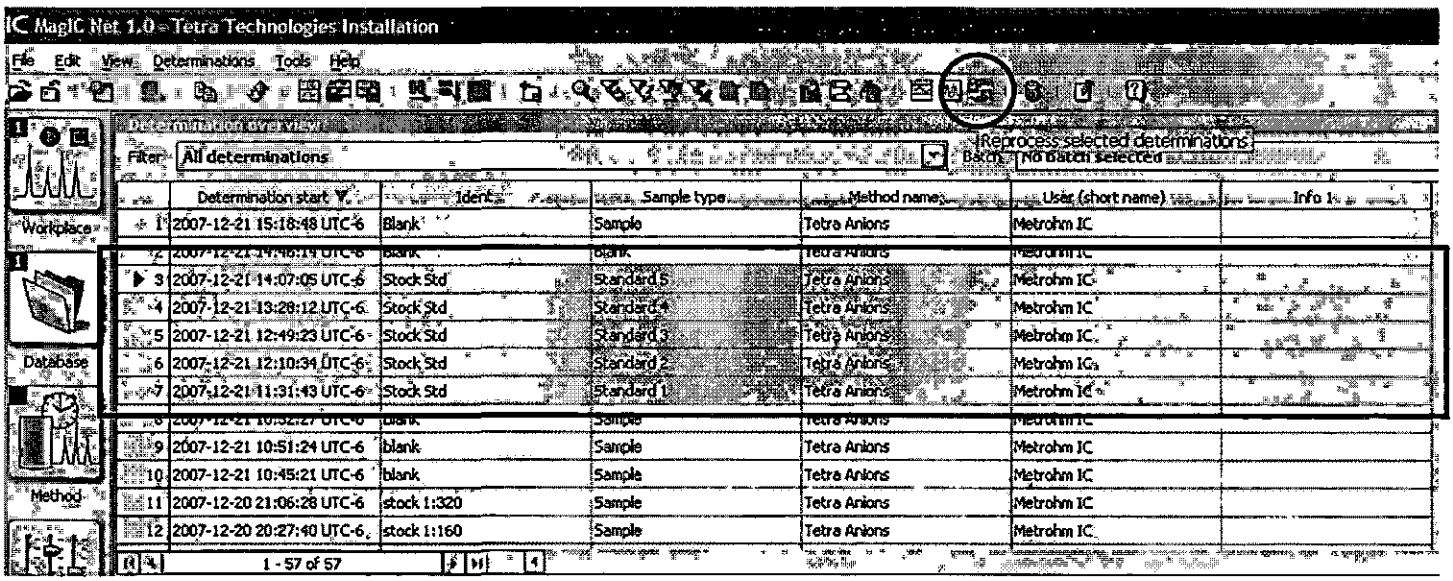
II. BASIC RECALIBRATION OF A METHOD (by batch reprocessing)

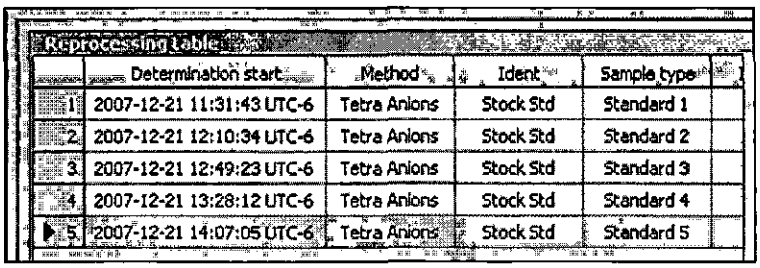
1. Equilibrate the instrument as detailed in **Section 2.2 System startup.**
2. Once the instrument is equilibrated, create a sample series as detailed in **Section 2.3 Starting a sample series.**
3. Start the sample series.

Update retention times

1. Click on the **Database** icon on the left side of the MagIC Net screen.

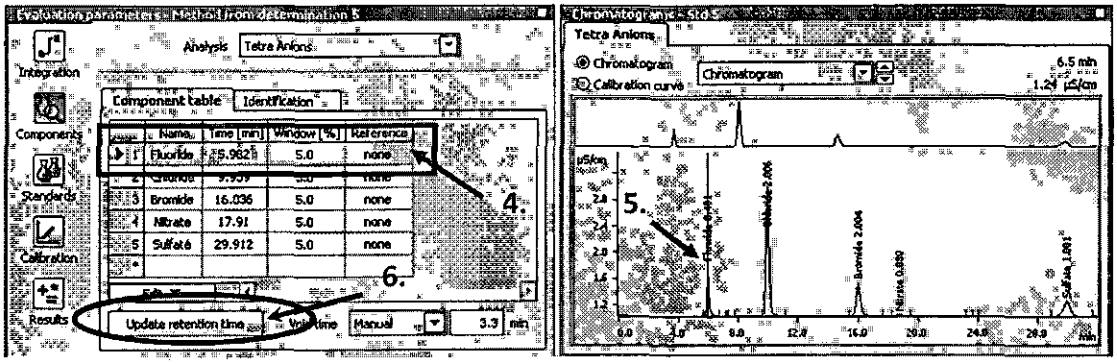
2. In the **Determination overview** highlight all of your standards and then click the **Batch reprocess button**  .





3. In the **Reprocessing table** select the highest standard (Standard 5).

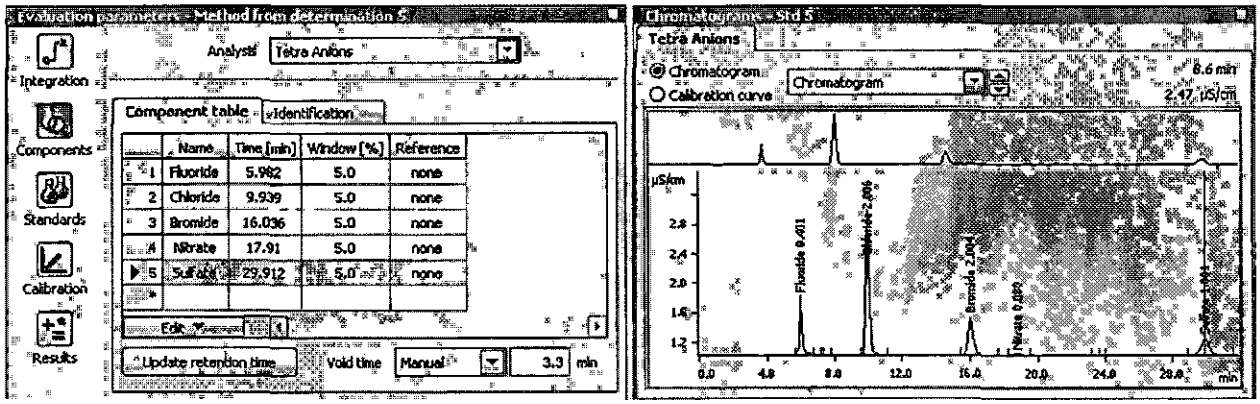
4. Left click on the line of the component table for the first analyte ion (Ex. Fluoride). This line of the component table will become highlighted in yellow.



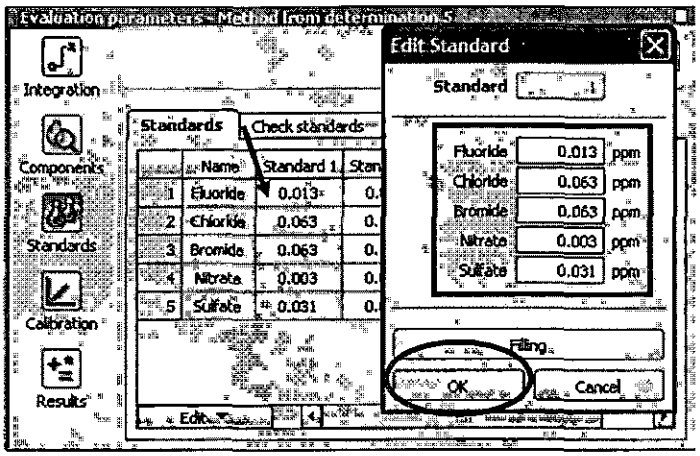
5. Now left click on the first peak of the **Chromatogram**; the peak will become highlighted in blue with the Retention time displayed in a pop-up box.

6. Once the first peak is highlighted, click the **Update retention time** button to update the stored retention time in the component table with the new retention time from the chromatogram on the left.

7. Repeat steps 4-6, clicking on each peak of the chromatogram and updating the retention time appropriately.



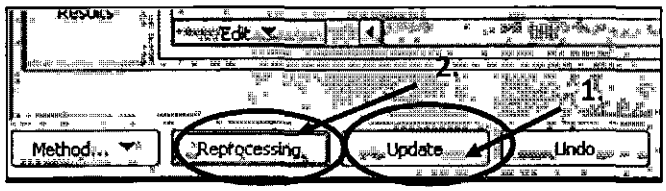
Update concentration values

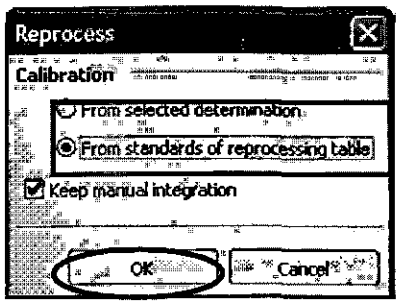


1. Click on the **Standards** button of the **Evaluation parameters**.
2. Double-left click on the column for Standard 1 to open the **Edit Standard** window. To change any of the standard values listed, click on the appropriate line and re-type the value. Click **OK** when finished.
3. Repeat steps 1-2 for each level in the standard table which needs to have concentrations updated.

Batch reprocess

1. After updating retention times and standard concentrations as shown above, click the **Update** button at the bottom left of the **Reprocessing** window.
2. Now click the **Reprocessing** button.

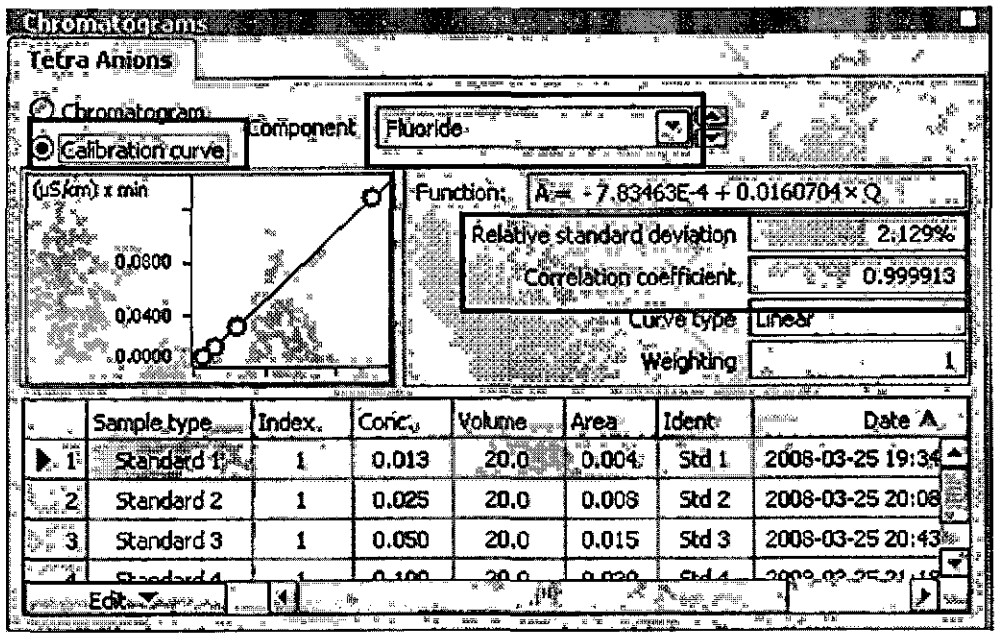


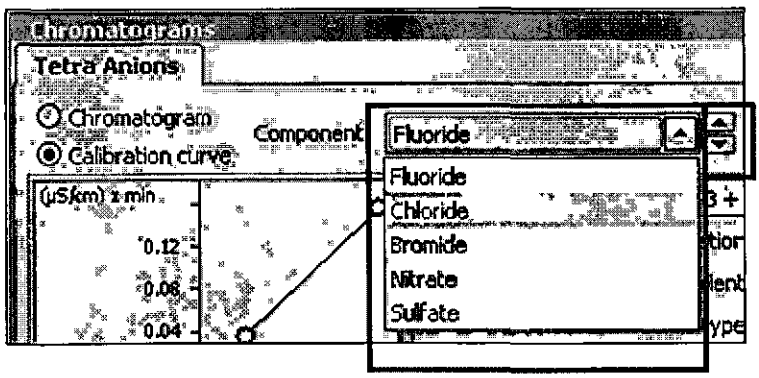


2. In the **Reprocess** window that appears, select "**From standards of reprocessing table**" and click **OK.**

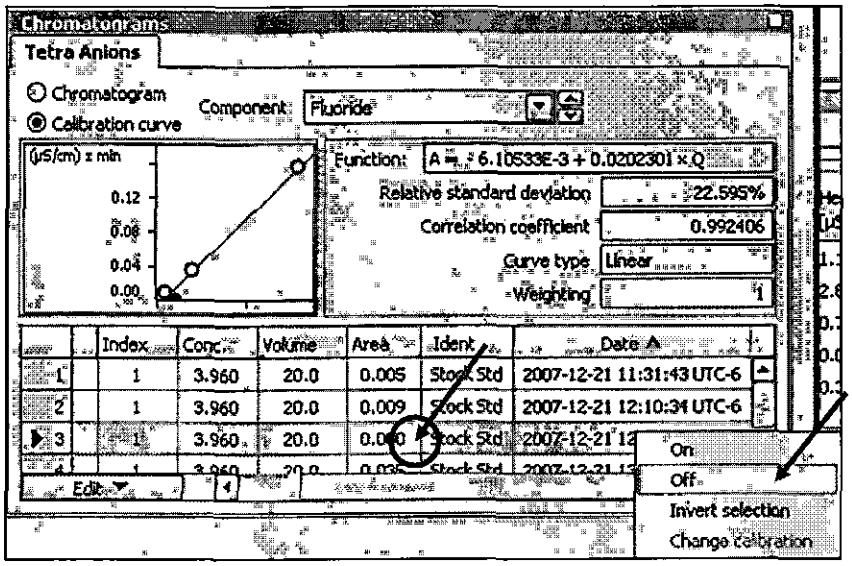
Calibration graph

1. To view the calibration graph that has been created by batch reprocessing, select **Calibration curve** in the **chromatogram** window. The calibration curve for the first analyte (Fluoride in this case) will be displayed. A suitable calibration should have a **Relative standard deviation** of 5% or less, and a **Correlation coefficient** of **0.999** or better.





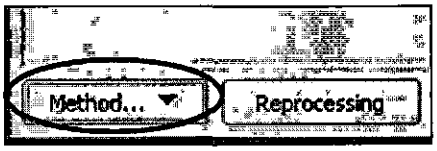
2. View the calibration graphs for other analytes by selecting them in the pull-down menu or by scrolling through them with the up and down arrows 



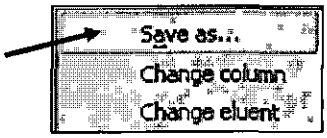
3. If a single point is throwing the calibration graph off, it can be excluded by right-clicking on one of the standards in the calibration table and selecting "**Off**".

4. Then click **Update** and **Reprocess** as described in steps 1-2 of Batch Reprocessing

Save calibration changes to the method

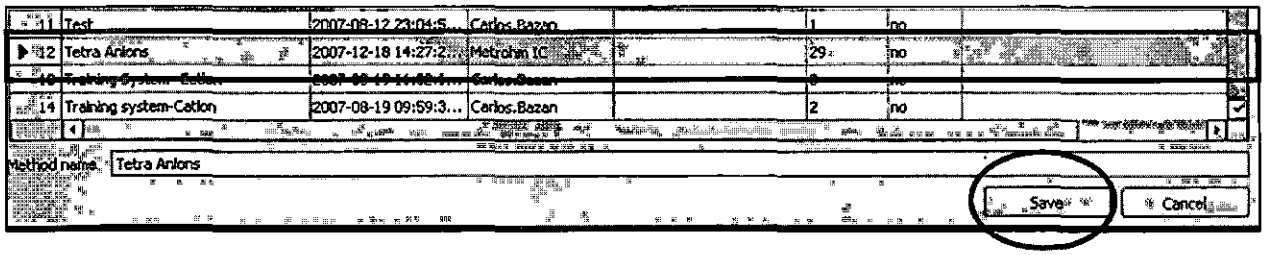


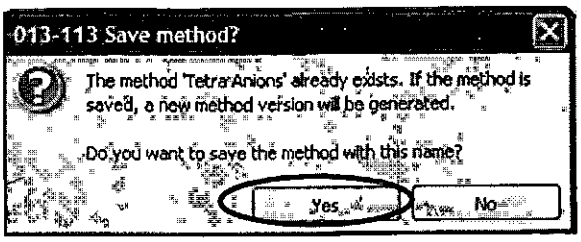
5. Click the **Method** button at the bottom left of the **Reprocessing** window.



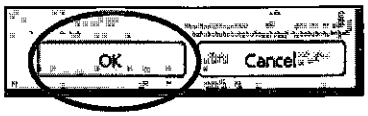
6. Select **Save as** in the pop-up menu. (Note that the Method *cannot be open in the Method window of MagIC Net while saving* changes from the reprocessing window or an error will occur. Close the method before continuing if necessary).

7. In the **Save method** window that appears, select the name of the method currently being used (Tetra Anions) and click **Save**.





8. Click **Yes** to save the method with this name (will overwrite the existing method with a new calibration).



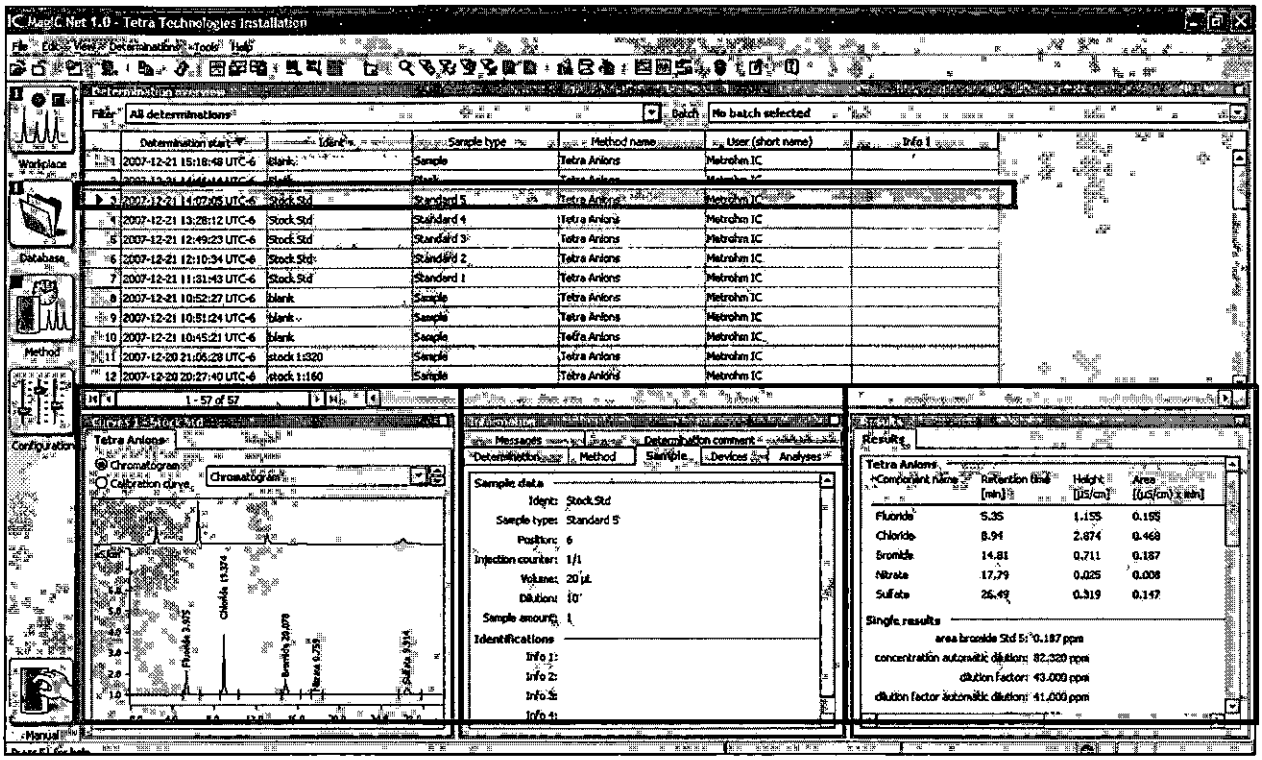
9. Click **OK** in the bottom right of the **Reprocessing** window to close it.

Once the reprocessing window is closed it will take a moment for the **Determination overview** to update with the reprocessed information.

2.6 Basic database navigation

Viewing Chromatograms in the Determination Overview

To view a chromatogram and its associated report information, select that line in the **Determination overview** of the **Database**.



Chromatograms are stored with the latest run at the top and earlier chromatograms towards the bottom of the series.

The following functions can be used to search or filter the determination overview according to a particular parameter:

Search the database for a particular sample **Ident** or other identifier.

Quick filter: Press this button to turn on the quick filter function. Whatever field you then highlight in the determination overview, and then double left-click on will then become the filter criteria.

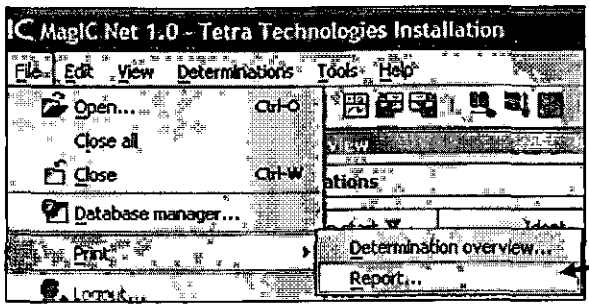
Define special filter allows you to select your own detailed filter criteria and apply it.

Apply last filter

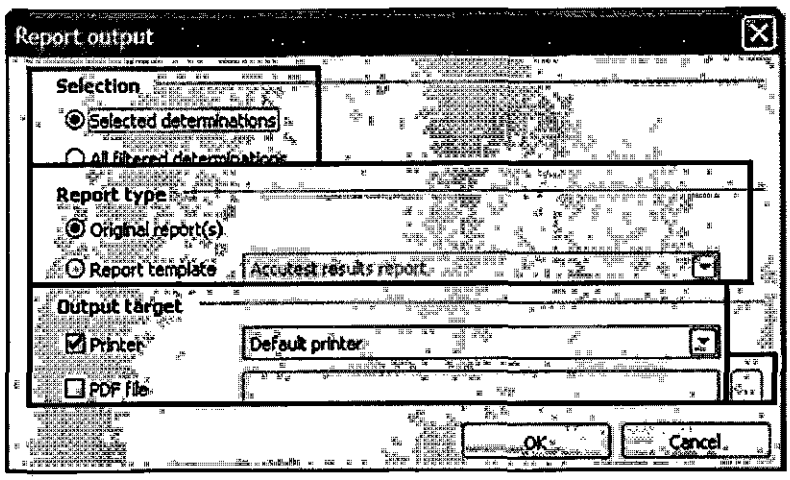
Remove applied filter returns the determination overview to its unfiltered condition.

2.7 Report Basics

1. Select one or more determinations to be printed by highlighting them in the **Determination overview** or by applying a filter.



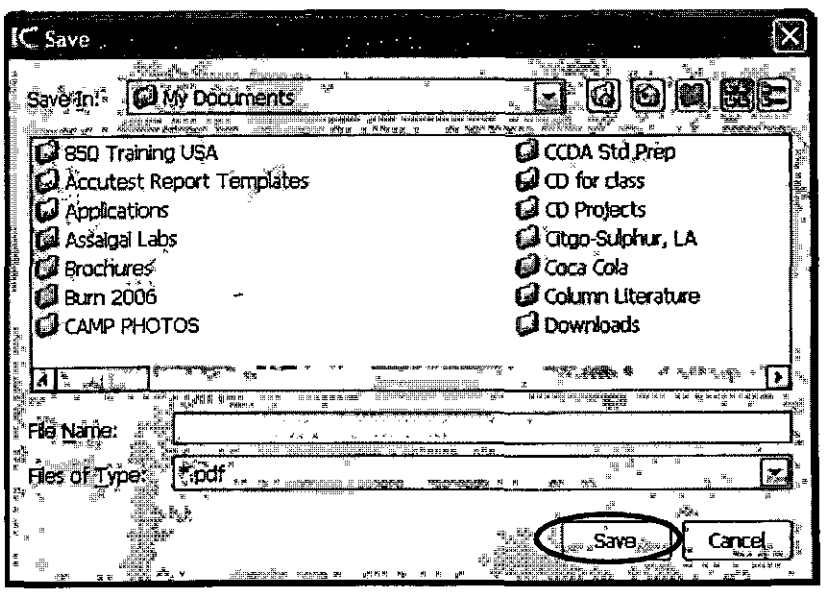
2. To print the report for a particular determination or determinations, highlight it in the **Determination overview** and then go to **File > Print > Report.**



3. Choose the **Selection** to be printed

4. Select whether the original report template will be used or to print the determinations with another report time (*original will be most* common).

5. Select the **Output target** (the printer to be used).

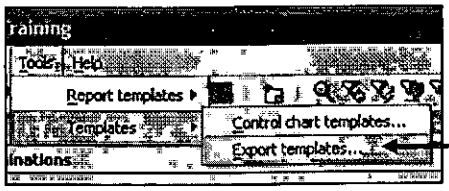


6. If desired, select the **PDF** option, and then press the [...] button to designate the file destination and file name and click **Save.**

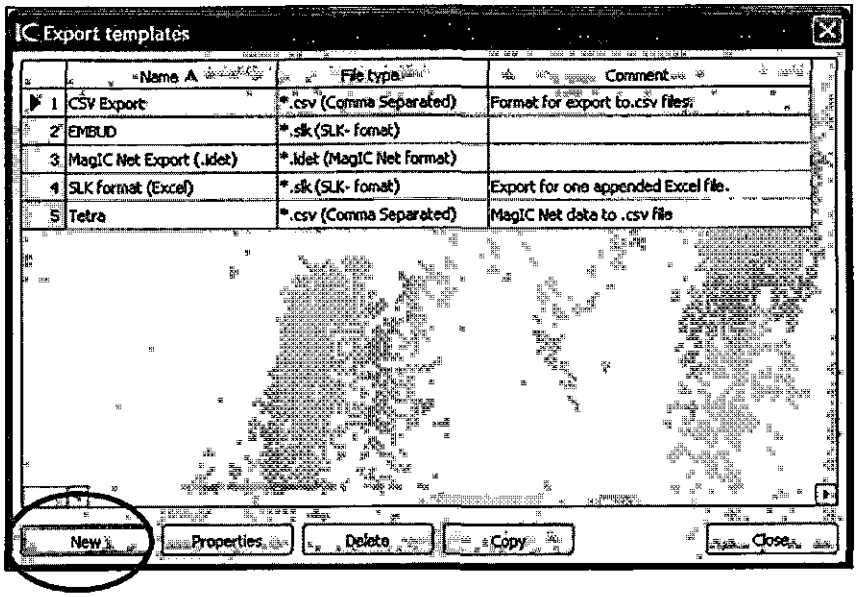
7. Click **OK** on the **Report output** window to send the reports to print and/or PDF.

2.8 E-mailing Chromatograms from MagIC Net

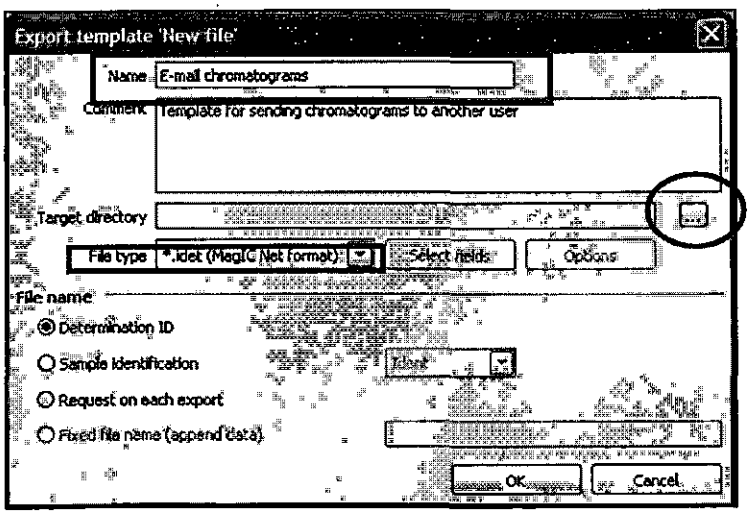
Creating an e-mail export template



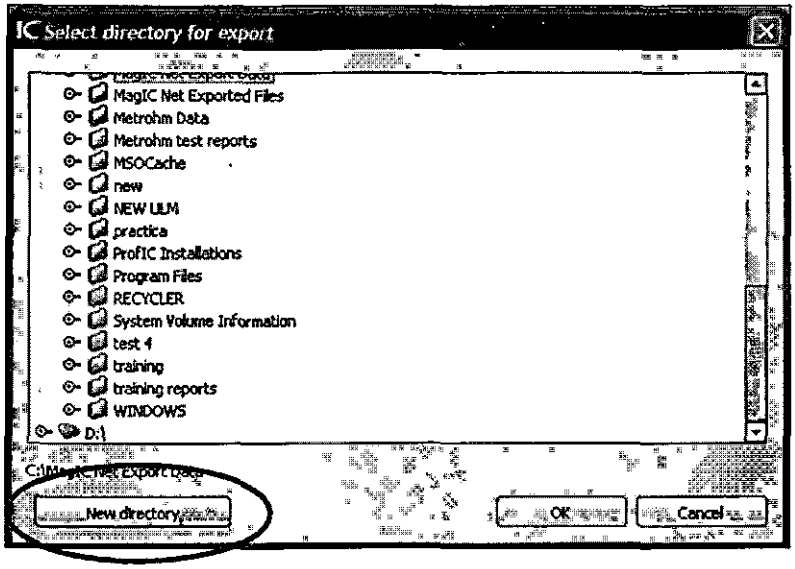
1. In the Database window go to the **Tools** directory and select **Templates > Export templates.**



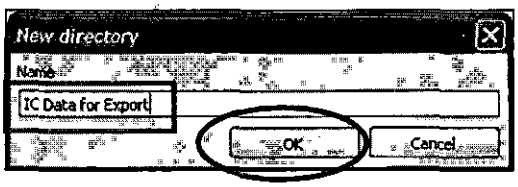
2. In the Export Templates window click on the **New** button.



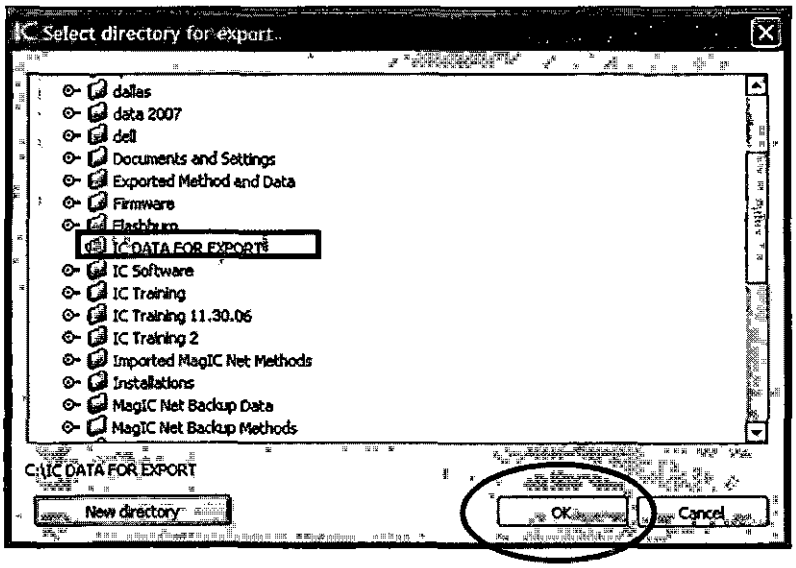
3. Name the template "**E-mail chromatograms**" or something similar.
4. Leave the **File type** set to ***.idet(MagIC Net format)**.
5. Click on the ... button to select the **Target directory** the template will send the files to.



6. Click the **New directory** button to create a distinct data directory for the exported files to go to.

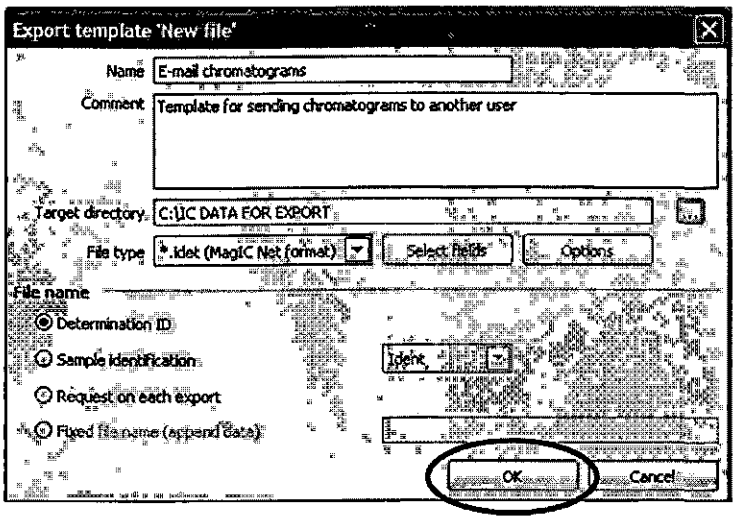


7. Give the directory a distinct name that you will easily remember (Ex. IC Data for Export), then click **OK**.

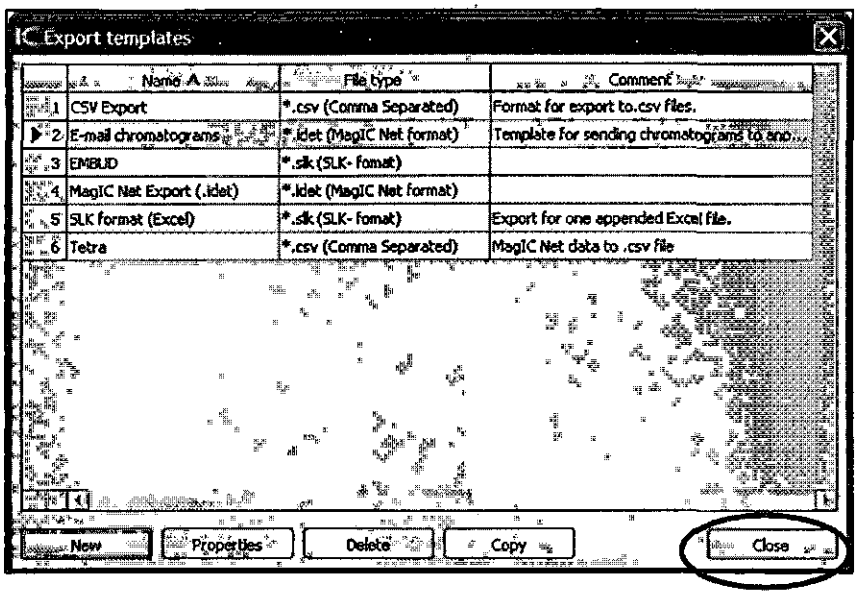


8. The new directory will now show up in the directory tree.

9. Click **OK** to finalize selection of the directory path.

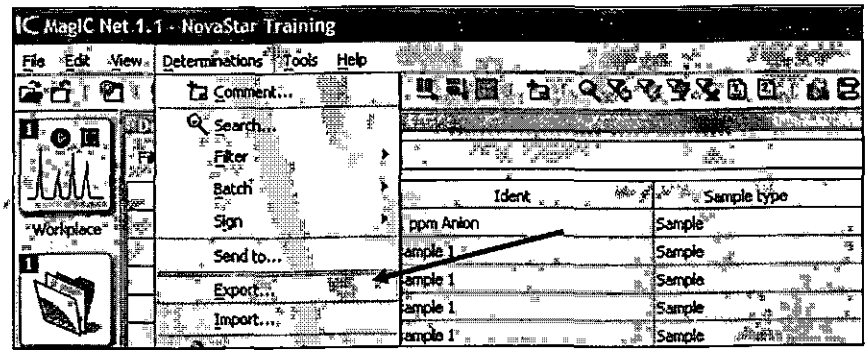


10. Click **OK** to complete creation of the new export template.

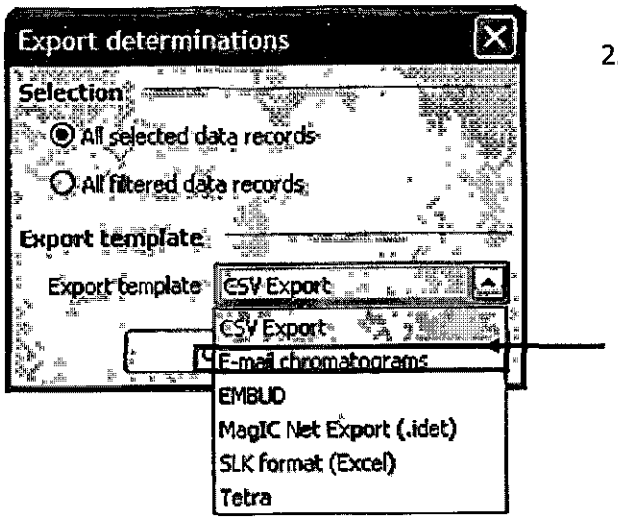


11. Click **Close** to exit out of the Export template window.

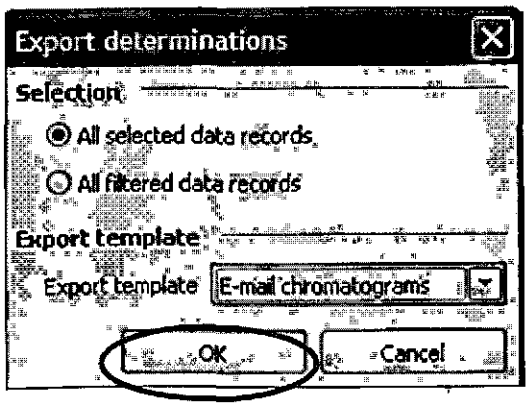
Exporting chromatograms to e-mail them



1. In the Database window highlight all the chromatograms you wish to e-mail, then select **Determination > Export.**



2. In the Export determinations window choose the selection "All selected data records" and then use the pull-down menu to select the appropriate export template (in this case "**E-mail chromatograms**).



3. Click the **OK** button on the Export determinations window to send the data to the Export folder designated in the template.

4. In your e-mail program, go to the feature that allows you to attach files to an e-mail message, navigate to the Export directory we designated in the Export template and select all the appropriate chromatograms you wish to e-mail.