CHEMIASOFT

Standard Curve

Software Manual

Revision 2

January 19, 2015

By

CHEMIASOFT TEAM

www.chemiasoft.com

Note: There might be some differences between this manual and the software due to continuous development. For the latest version of this manual please refer to online version.

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About

Standard Curve is defined as the easiest way to graph calibration curve from standard solutions and identify unknown samples in laboratory. There is no need to use MS Excel to make calculations and pain full process. **Standard Curve** made it easy for you.

Calibration is at the heart of chemical analysis, and is the process by which the response of an instrument (in metrology called ‘‘indication of the measuring instrument’’) is related to the value of the concentration of the analyte.

A typical example in analytical chemistry is the calibration of a GC (gas chromatography) analysis. The heights of GC peaks are measured as a function of the concentration of the analyte in a series of standard solutions (‘‘calibration solutions’’) and a linear equation fitted to the data.

Standard Curve is robust industrial productivity software. It has been developed in real laboratory world. Width **Standard Curve**, laboratory routine work becomes easy. In addition, all data will be saved in local computer database and it can be backed up at anytime.

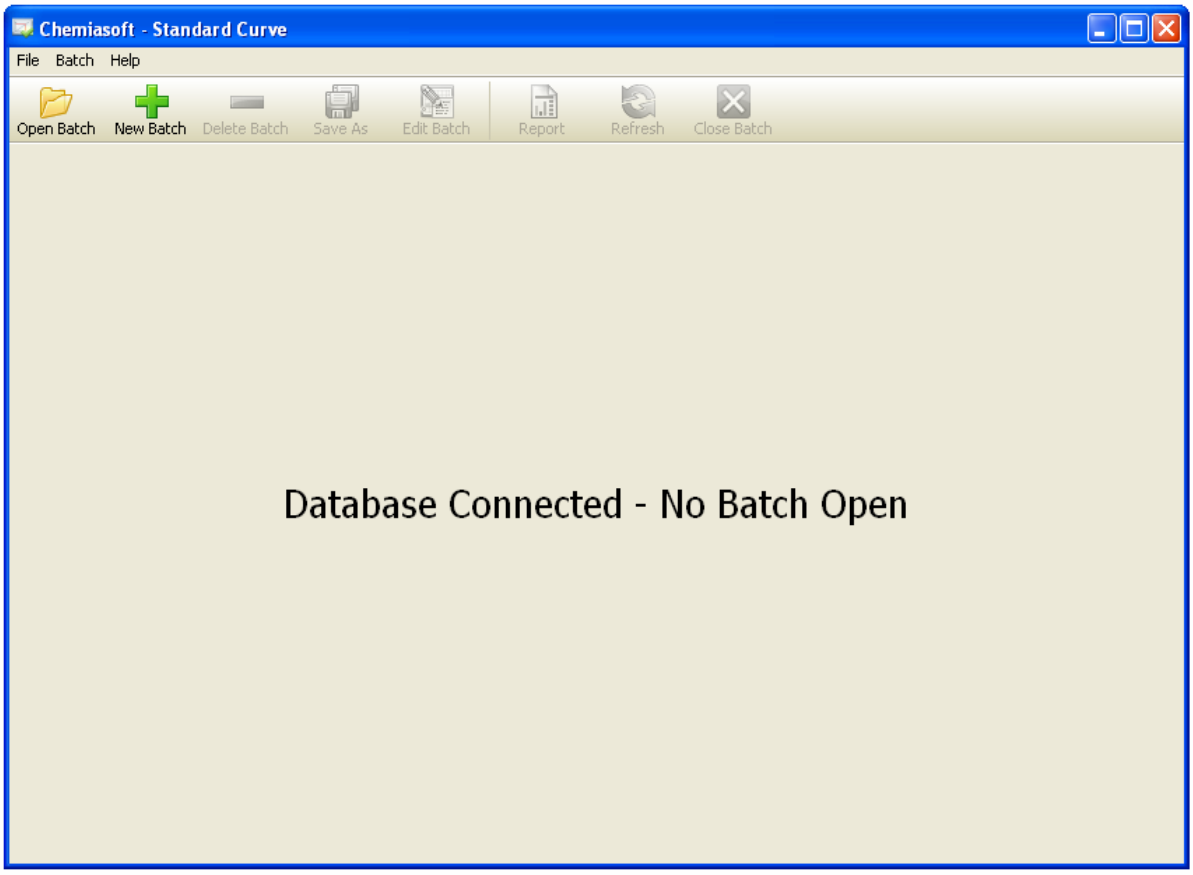
Start using **Standard Curve** today and make your life easy.

Features

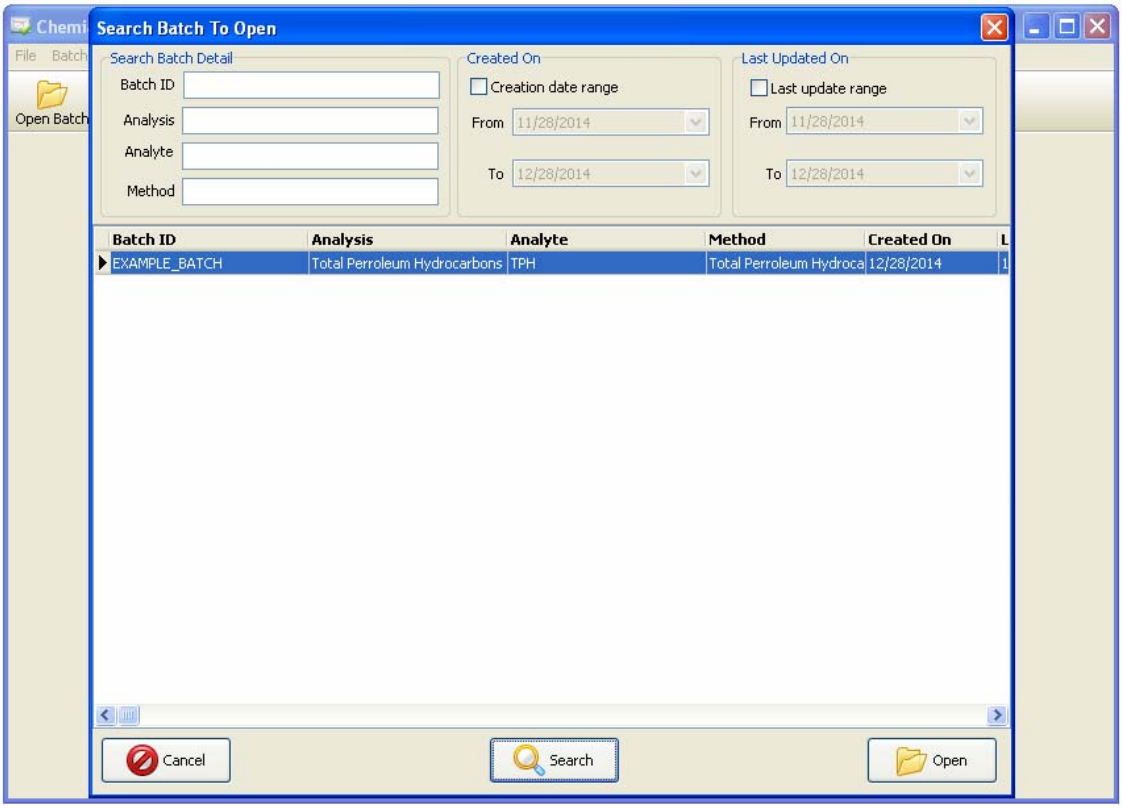
- Easy to use and straight forward.
- Support MS Access database.
- Create unlimited number of batches. Every batch includes calibration curve and unknown samples.
- Graph and run calibration curve from standard solutions and identify unknowns.
- Several types of trend line fitting include (Linear, Quadratic, Logarithmic base 10, Exponential, Power and Natural Logarithmic).
- Support both **O**rdinary **L**east **S**quare (**OLS**) and **W**eighted **L**east **S**quare (**WLS**) calibration methods.
- Accept single or multiple measurement values (like absorbance, peak area or peak height) and calculate average and RSD.
- Include or exclude standards from calibration curve.
- Graph calibration points and trend line.
- Display calibration result in table (like fitting equation, standard errors for equation parameters, coefficient of determination and standard regression error (also called residual standard deviation).
- Calculate concentration of unknown samples based on calibration curve.
- Support several multiplication factors to finalize calculation in origin samples. For example (Dilution factor, total volume and initial sample weight).
- Calculate method detection limits (MDL) as per ISO-11843-2, Hubaux & Vos and SEMI standard method.
- Set quantification limits and final reporting limits.
- Generate professional batch report, includes standards, calibration curve and unknowns.
- Export report as PDF, MS Excel, Image and Email and other formats.
- Print and export graph as PDF and image.
- Search batches using several inputs like batch ID, analyte, analysis, method, creation date and modification date.
- Delete and restore batches

Getting Started

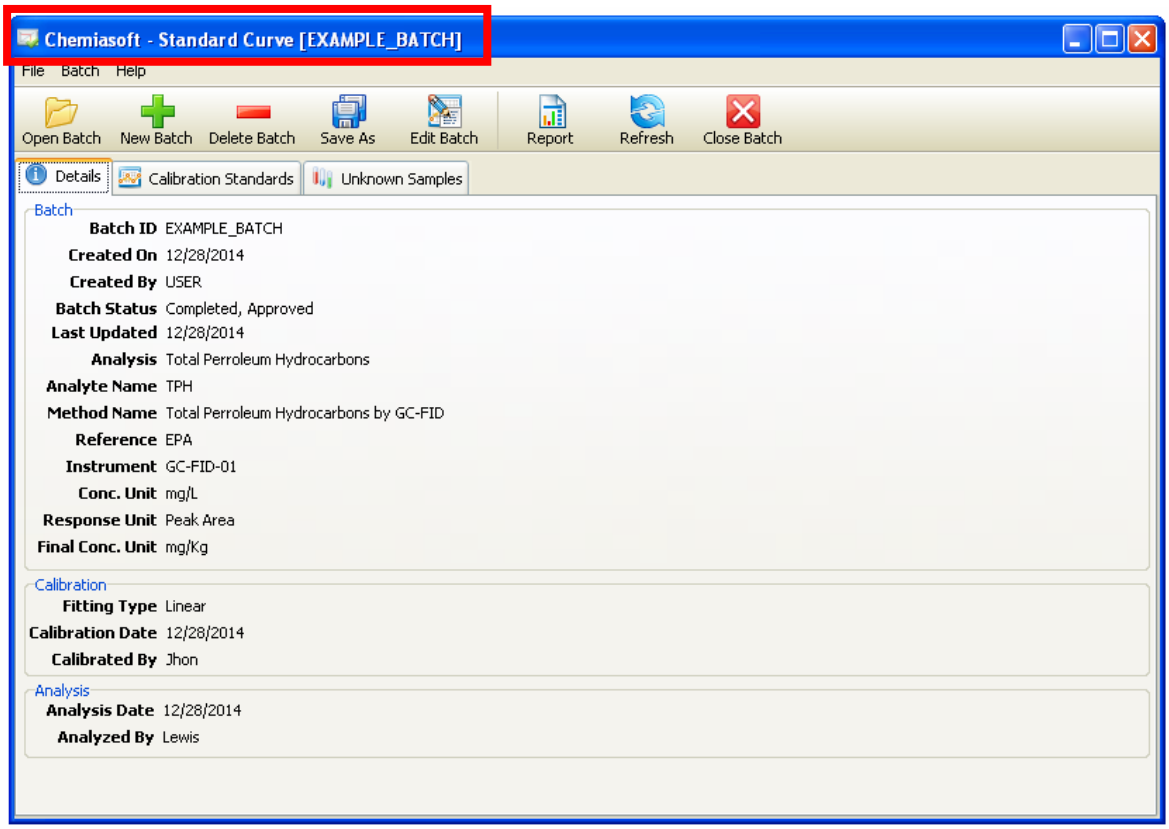
1. After installation of the software complete, run **Standard Curve** from desktop icon or from start menu. Once the software start, it will connect to local default database and the main software screen will appear



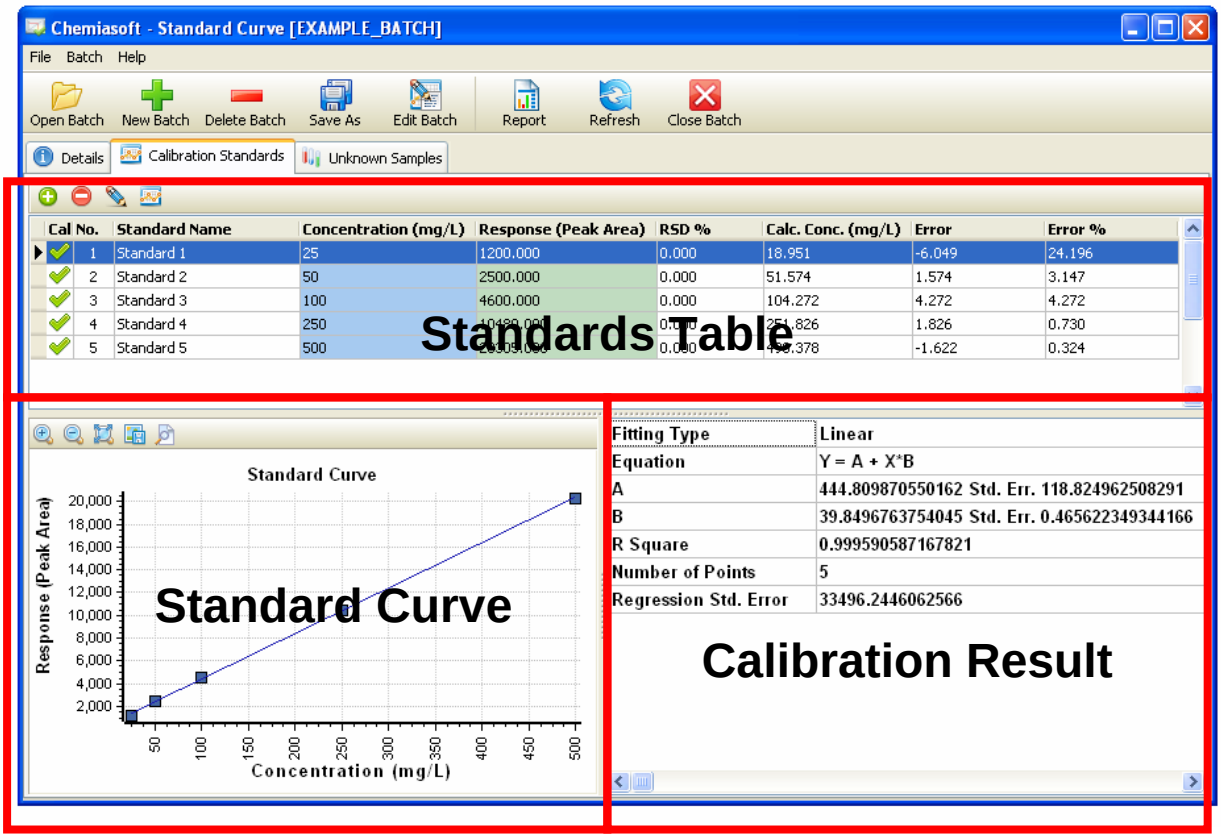
2. Once the main screen appeared, it will show "**Database Connected**". If there is any problem with database then refer to Database section.
3. Now press **Open** button on the main toolbar and search dialog will appear.
4. Leave all fields empty and press **Search** button. List of all available batches will appear.



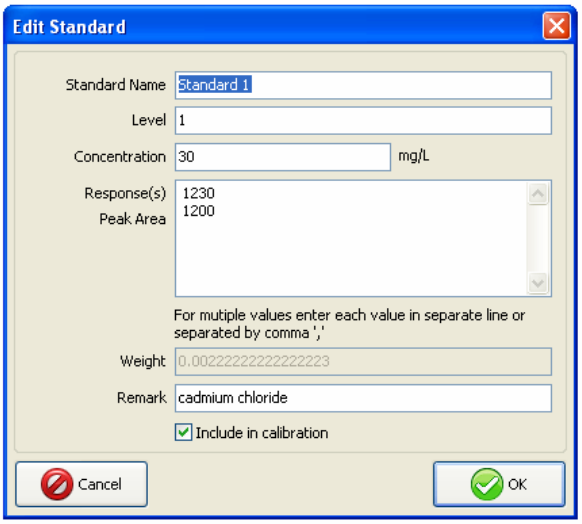
5. Double click on **EXAMPLE_BATCH** to open.
6. After selected batch open, main batch screen will appear. Batch name will show at title bar of the software between two brackets [EXAMPLE_BATCH].



Batch screen contains three tabs (**Details**, **Calibration Standards** and **Unknown Samples**). The Details tab contains information about the batch. Now switch to **Calibration Standards** tab.



7. On **Calibration Standards** tab screen become three parts, **Standards** table at the top which list all calibration standard solutions, **Standard curve** area at the left bottom shows the calibration curve. On the bottom right area there is **Calibration Result** table which contains fitting type, equations and other details related to calibration.
8. On **Standards** table, the first column "**Cal**" shows tick mark when the standard included in the calibration.
9. On the Standards table, double click on the standard 2 row. The dialog will appear as follow.

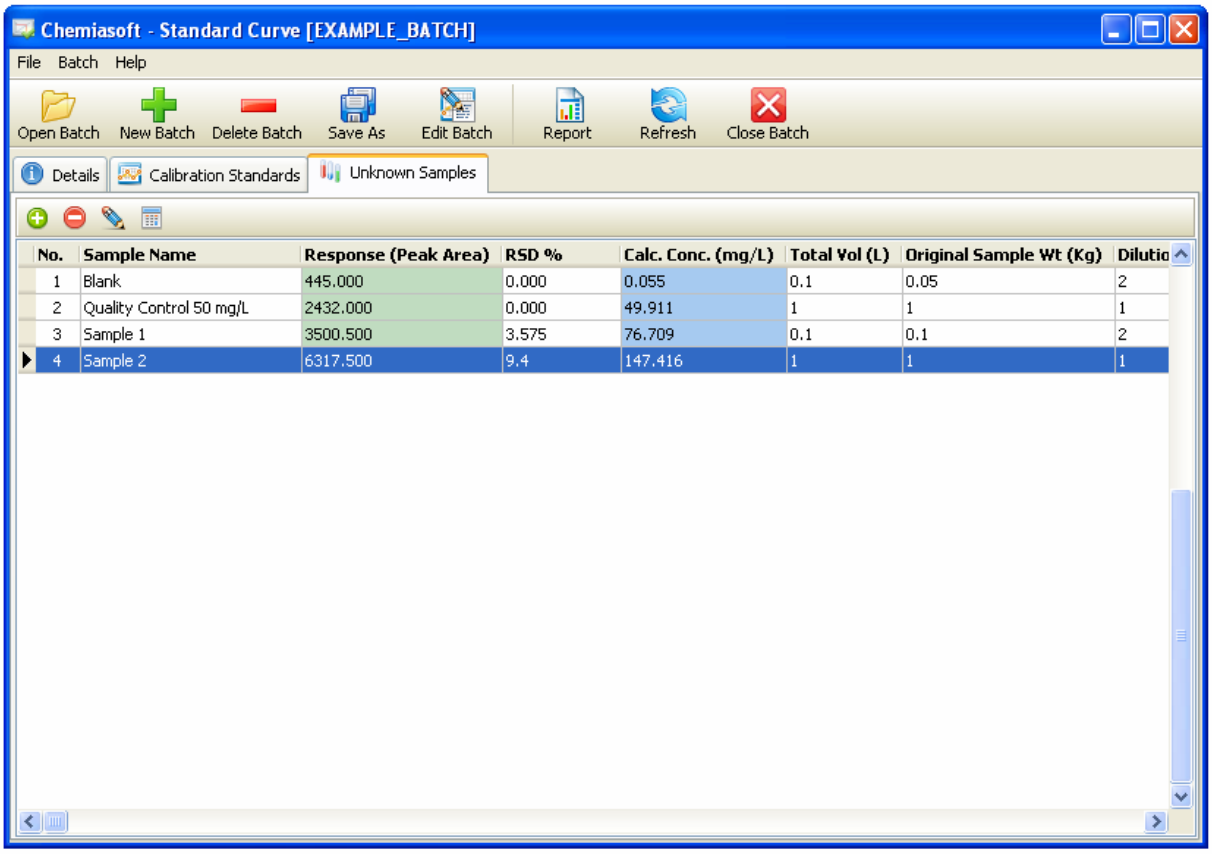


On **Edit Standard** dialog, there are several input fields include **standard name**, **level**, **remark**, **concentration** and **responses**. The concentration must be single value, but responses can accept several values by separate them with comma or enter each value in new line. The software will calculate average of all entered response(s) and calculate relative standard deviation (RSD).

Weight value required when using weighted calibration (WLS) and manual entry of weight factor.

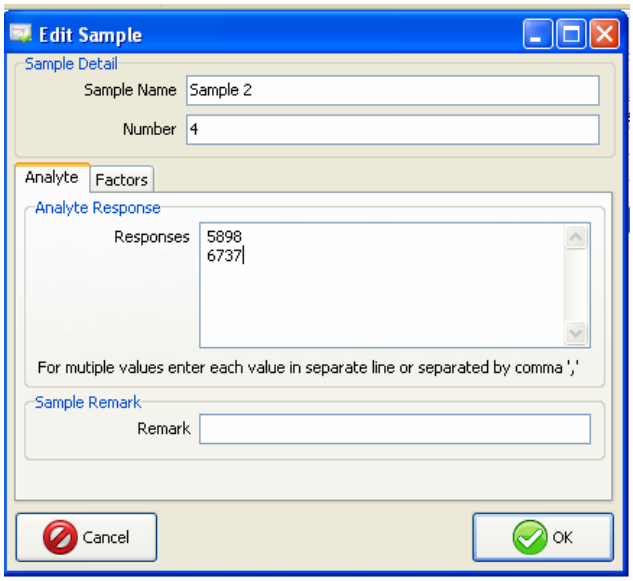
"**Include in calibration points**" to include or exclude standard from calibration curve. Uncheck the box to exclude from calibration and press **OK** to see the effect. Equation will be recalculated. All samples also will be recalculated base on new fitting.

10. Switch to **Unknown Samples** tab, table contains all samples in the batch with their responses and calculated concentrations

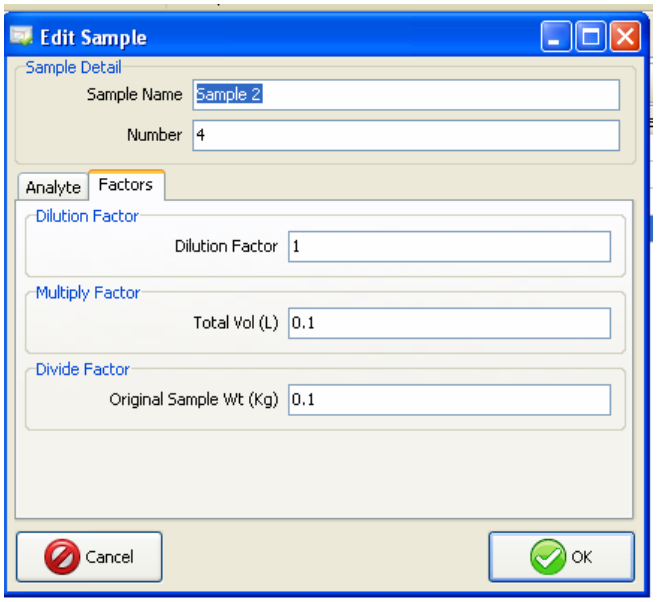


No.	Sample Name	Response (Peak Area)	RSD %	Calc. Conc. (mg/L)	Total Vol (L)	Original Sample Wt (Kg)	Dilutio
1	Blank	445.000	0.000	0.055	0.1	0.05	2
2	Quality Control 50 mg/L	2432.000	0.000	49.911	1	1	1
3	Sample 1	3500.500	3.575	76.709	0.1	0.1	2
4	Sample 2	6317.500	9.4	147.416	1	1	1

Double click on any sample by left mouse click, **Edit Sample** dialog will show up



The dialog contains sample input details, like (**sample name**, **order number** and **responses**) similar to the standards dialog. In addition, it contains **Factors** tab, click on factors tab to see the details.

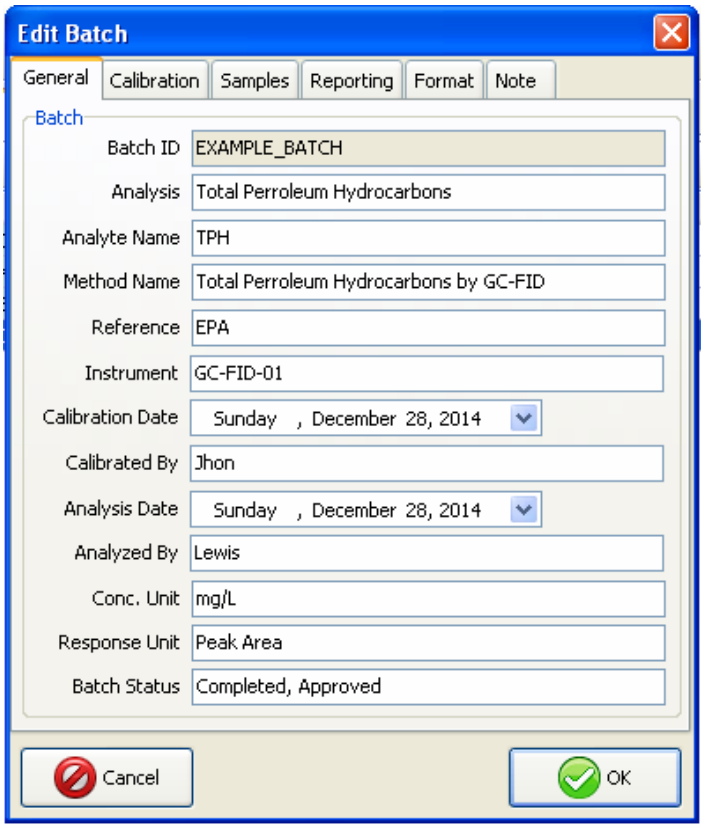


Different factors are appeared. **Dilution Factor,** how many times sample is diluted. **Total volume**, the total sample solution in liter. **Origin Sample Weight** the amount of the sample in sample preparation process in kilograms.

The factors are very essential in lab calculations. In this example, calculated concentration from calibration curve in mg/L will be multiplied by dilution factor and then multiplied by total volume of the sample solution. The result will be divided by origin sample weight (Kg) in this example 100 g = 0.1 Kg. The final calculated value will be in mg/kg, which is the concentration of the analyte in origin sample. (i.e. the reported concentration).

Click **OK** or **Cancel** button to hide **Edit Sample** dialog.

11. On the toolbar click on **Edit Batch** button. Edit batch dialog will appear



Edit Batch dialog contains all information about the batch and calibration. At the top there are several tabs, you can switch between tabs and discover the details. Make some changes and press **OK** button to see the effect.

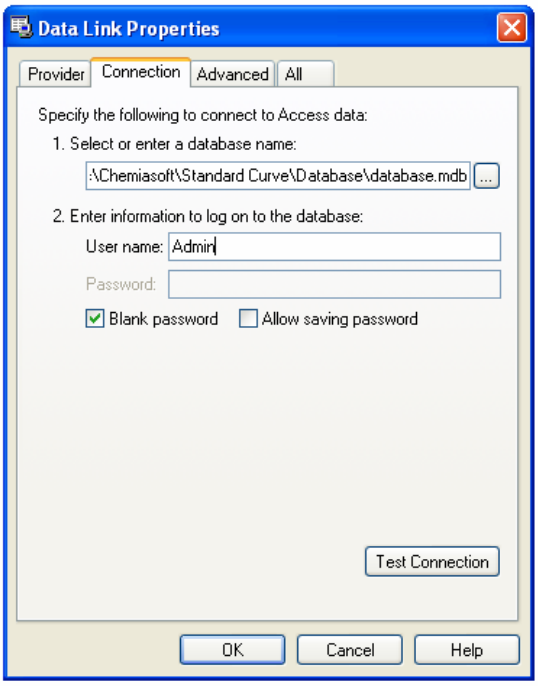
That is all for now. Please refer to the **Table of Content** (page 2) and find out more details. If you can't find answer of your question, please contact us by sending an email to support@chemiasoft.com

Database

Standard Curve software is database software. It is supporting **MS Access** database. Future versions will be developed to support other types of databases Like MySQL.

The default database is located in:
C:\Program Files\Chemiasoft\Standard Curve\Database\database.mdb

To change database properties go to menu **File >> Database Properties**. **Data Link Properties** dialog will show up. Change database properties or location then press **OK**.

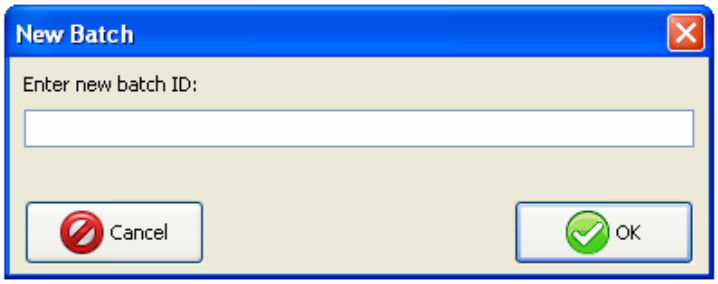


Batches

In **Standard Curve** software, every collection of calibration standards and unknowns called a "**batch"**.

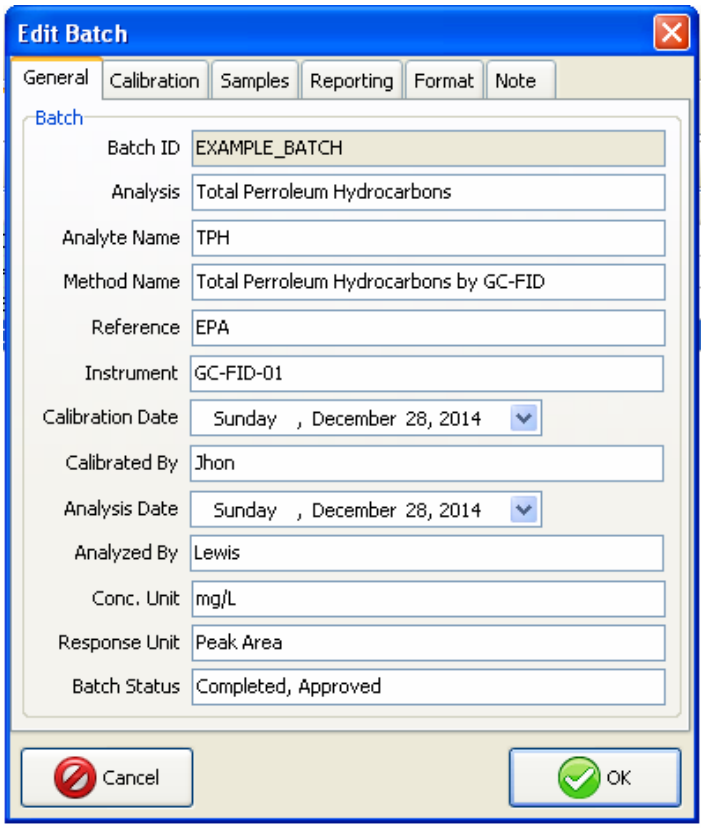
Create New Batch

To create new batch, from toolbar click **New Batch** button, enter a unique name of the batch and press **OK**.



If the batch name is unique, the name will be reserved in the database. It is preferred to have unique naming system of all batches in lab. For example, use batch name derived from date of analysis like if a batch analyzed on Jan, 8, 2015 will be named as (e.g. B20150108-A), B means batch and A means first trial of analysis performed. **Be careful** batch name is permanent and can not be changed after created.

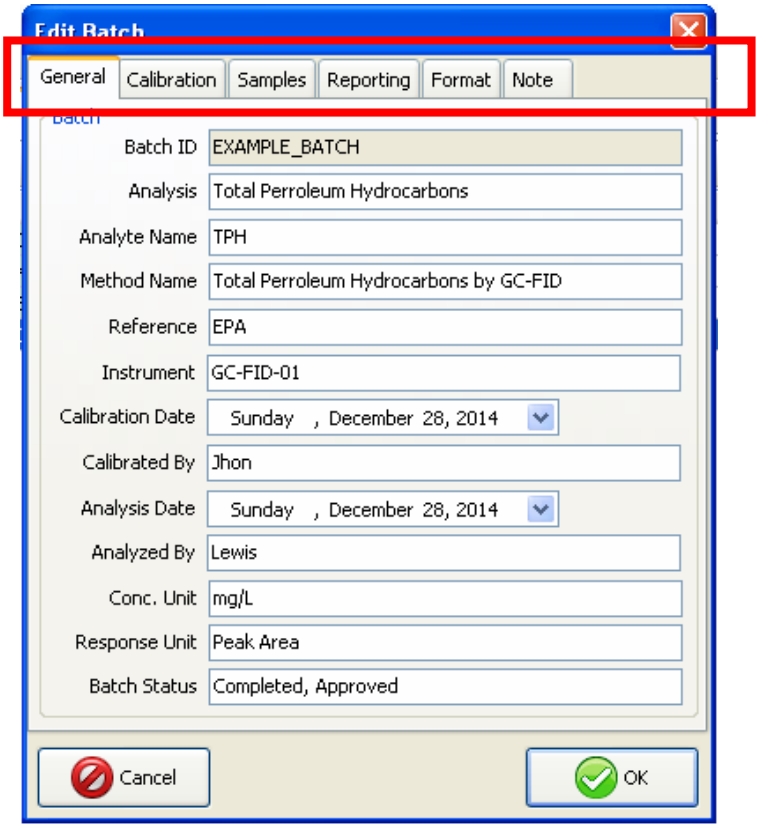
Once you press OK, **Edit Batch** Dialog will appear.



Fill batch information and press **OK**.

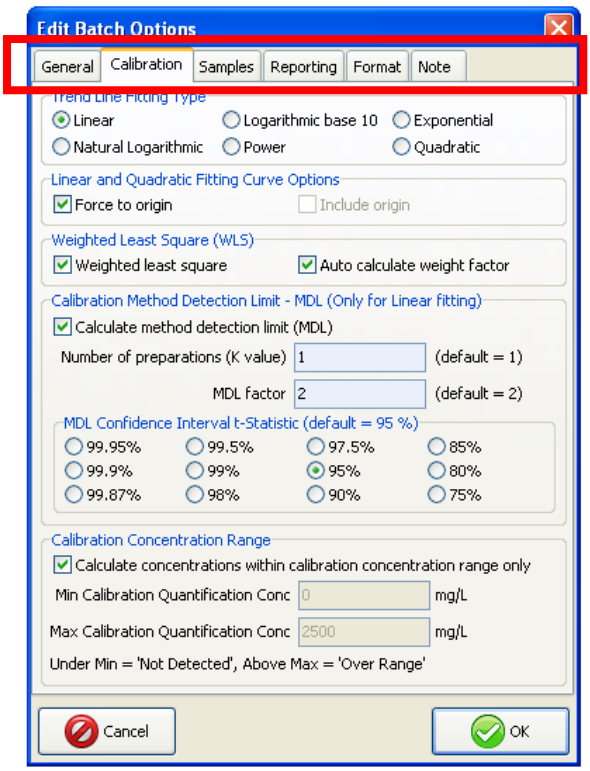
Edit Batch Options

To edit batch options click on **Edit Batch** button. Edit Batch dialog will appear



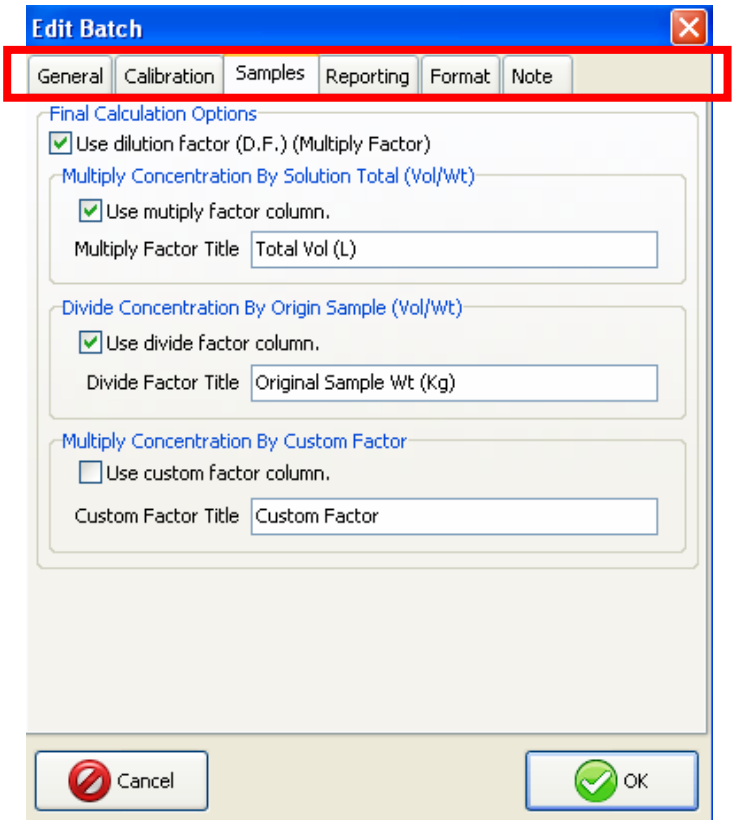
Edit Batch dialog contains several tabs and below is the details of each:

General Tab	
Item	**Description**
Batch ID	Unique batch ID in the database. This field is “read only”. It can’t be changed after it has been created.
Analysis	Analysis name which is performed in the lab (e.g. Hydrocarbons, Chloride, Sulfate…etc).
Analyte Name	Name of the analyte to be analyzed
Method Name	The laboratory method name or standard operation procedure (SOP)
Reference	Reference method number (e.g. EPA, ASTM, ISO…etc)
Instrument	Instrument name or ID used to perform analysis and read analyte responses (e.g. UV-VIS, HPLC, GC, ICP…etc)
Standard Solvent	Solvent name used to dilute standard solutions.
Sample Solution	Solvent name used to dilute sample solutions.
Calibration Date	Date of the calibration run of the standards
Calibrated By	Name of the analyst perform the calibration process
Analysis Date	Date of performing sample analysis
Analyzed By	Name of the person perform sample analysis
Solns. Conc. Unit	Concentration of the solutions used in the analysis including both calibration solutions and samples solutions.
Response Unit	Response name from the instrument used to perform the analysis (e.g. Peak Area, Peak height, Absorbance, intensity…etc).
Batch Status	Status of the batch (e.g. Under process, under review, rejected, approved…etc).



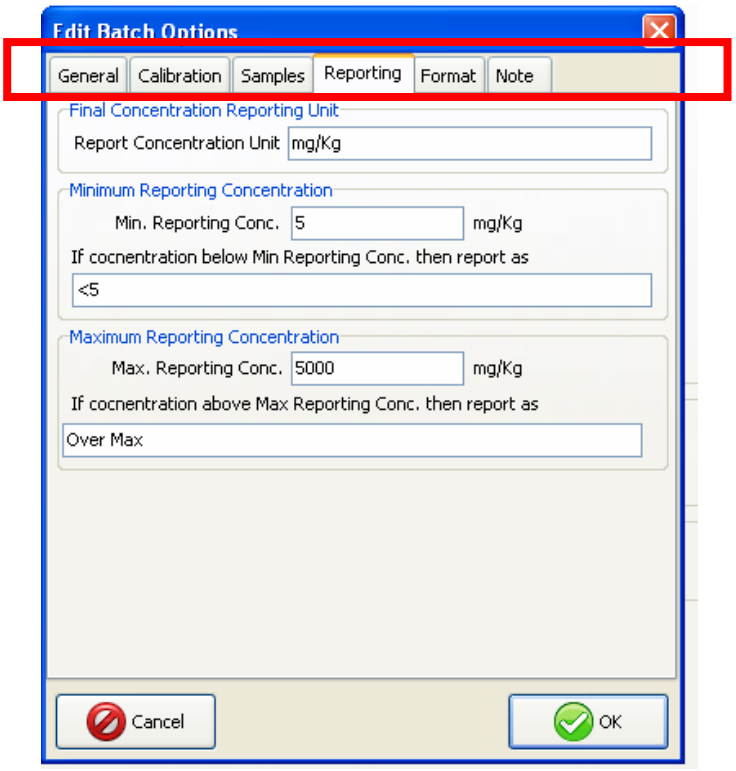
Calibration Tab	
Item	**Description**
Trend Line Fitting Type	Fitting type, there are six options available (Linear, Power, Natural Logarithmic, Logarithmic base 10, exponential and Quadratic)
Fitting Curve Options	**Force To Origin**, make fitting line pass through origin point (0,0) this option available only for quadratic and linear type. **Include Origin**, include origin point (0,0) to the calibration points.
Weighted Least Square (WLS)	Select **Weight Least Square (WLS)** option to enable weighted calibration. When this option is not selected, **Ordinary Least Square (OLS)** will be used in calculations.
Method Detection Limit	Calculate method detection limit (MDL) for batch calibration. Enable this option when batch is conducted for MDL study. MDL is calculated according to ISO 11843-2 “Methodology in the linear calibration case”, also called “Hubaux Vos MDL”. Refer to those methods online for more details on how to calculate MDL. Set **K value**, **MDL factor** and **Confidence Interval** as per method requirement.
Calibration Concentration Range	Two options are available here: • When **Report within Calibration Range** is checked then only samples solutions concentration within calibration range will be reported. If sample solution below calibration range, it will be reported as “**Under Range**” or “**Over Range**” if exceed calibration range concentration. The concentration range will be identified automatically by identify the maximum and minimum concentration in the calibration standards. • When uncheck **Report within Calibration Range** then you have to enter quantification concentration range. Enter maximum and minimum calibration quantification

Calibration Tab	
Item	**Description**
	concentration to be determined base on the equation. *Note*: **Calibration range** is different from **Final reported range** (shown in **Report** tab). **Calibration range** is defined as the analyte concentrations in solutions used during running instrument and take reading (responses). **Final reported range** is defined as the concentration of analyte in origin sample. Reported concentration is calculated from solution concentration.

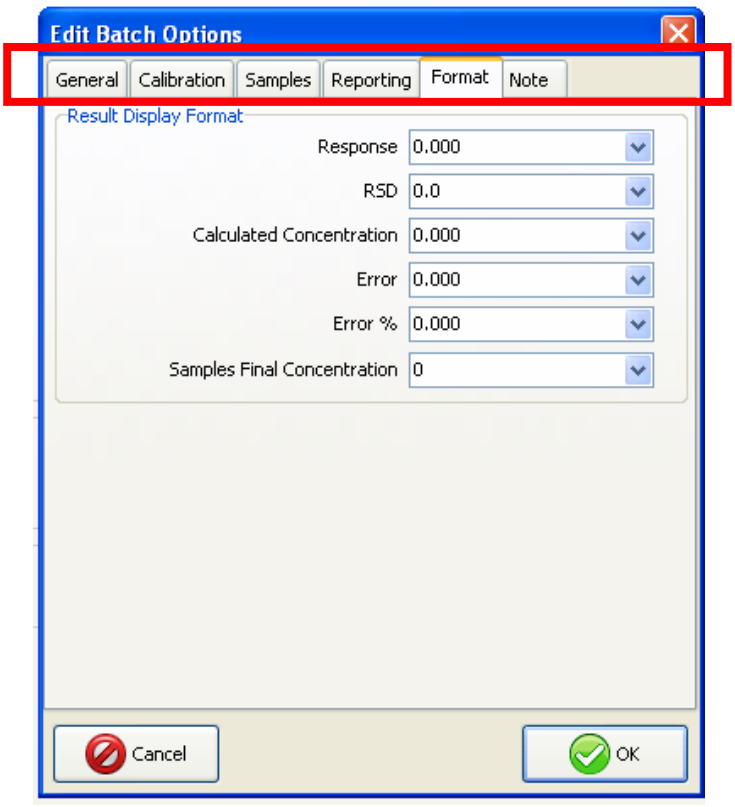


Samples Tab	
Item	**Description**
Use dilution factor	Check this option to include dilution factor column in samples table. This part is very essential when you have high concentrated samples and you want to make dilution before injected to the instrument. Dilution factor is calculated using equation: $$\mathrm{DF} = \frac{\text{Final Volume (mL)}}{\text{Initial Volume (mL)}}$$ For example if you take 5 mL from solution and diluted to 100 mL with solvent then dilution factor will be: $$\mathrm{DF} = \frac{100\,(\mathrm{mL})}{5\,(\mathrm{mL})} = 20$$
Multiply Factor	Check this option to include multiply factor column in samples table. This will multiplied calculated concentration by this factor. Mostly used when sample required preparation before analysis, like digestion in trace metal analysis. For example enter "**Total Volume (L)**" in the title field.
Divide Factor	Check this option will include divide factor column in samples table. This will divide calculated concentration by this factor. Mostly used when sample required preparation before analysis, like digestion in trace metal analysis. For example enter "**Sample Weight (Kg)**" in the title field.

Samples Tab	
Item	**Description**
Custom Factor	Check this option to include custom multiply factor column in samples table. This will multiplied calculated concentration by this factor. This factor is considered as extra option. Use it if you want to make correction factor of the calculated concentration. For example conversion factor from Liter to milliliter…etc.



Reporting Tab	
Item	**Description**
Reporting Concentration Unit	The final concentration unit after performing all calculations.
Min. Reporting Conc.	The minimum reporting concentration of the original sample.
If concentration below Min. Reporting Conc. Then report as	Enter the text to be reported if the final calculated concentration below Min. Reporting Conc.
Max. Reporting Conc.	The maximum reporting concentration of the original sample.
If concentration above Max. Reporting Conc. Then report as	Enter the text to be reported if the final calculated concentration above Max. Reporting Conc.



Format Tab

In this tab, set details of digital value format to display result in standards and samples tables as per your needs. The following format specifiers are supported in the format result:

Specifier	Represents
0	Digit place holder. If the value being formatted has a digit in the position where the '0' appears in the format result, then that digit is copied to the output result. Otherwise, a '0' is stored in that position in the output string.
#	Digit placeholder. If the value being formatted has a digit in the position where the '#' appears in the format string, then that digit is copied to the output string. Otherwise, nothing is stored in that position in the output string.
.	Decimal point. The first dot character ('.') in the format string determines the location of the decimal separator in the formatted value; any additional dot characters are ignored. The actual character used as the decimal separator in the output string is determined by the DecimalSeparator global variable, whose default value is specified in the Number Format of the International section in the Windows Control Panel.
,	Thousand separator. If the format string contains one or more comma characters (','), the output will have thousand separators inserted between each group of three digits to the left of the decimal point. The placement and number of comma characters in the format string does not affect the output, except to indicate that thousand separators are wanted. The actual character used as the thousand separator in the output is determined by the ThousandSeparator global variable, whose default value is specified in the Number Format of the International section in the Windows Control Panel.

The following table shows some sample formats and the results produced when the formats are applied to different values:

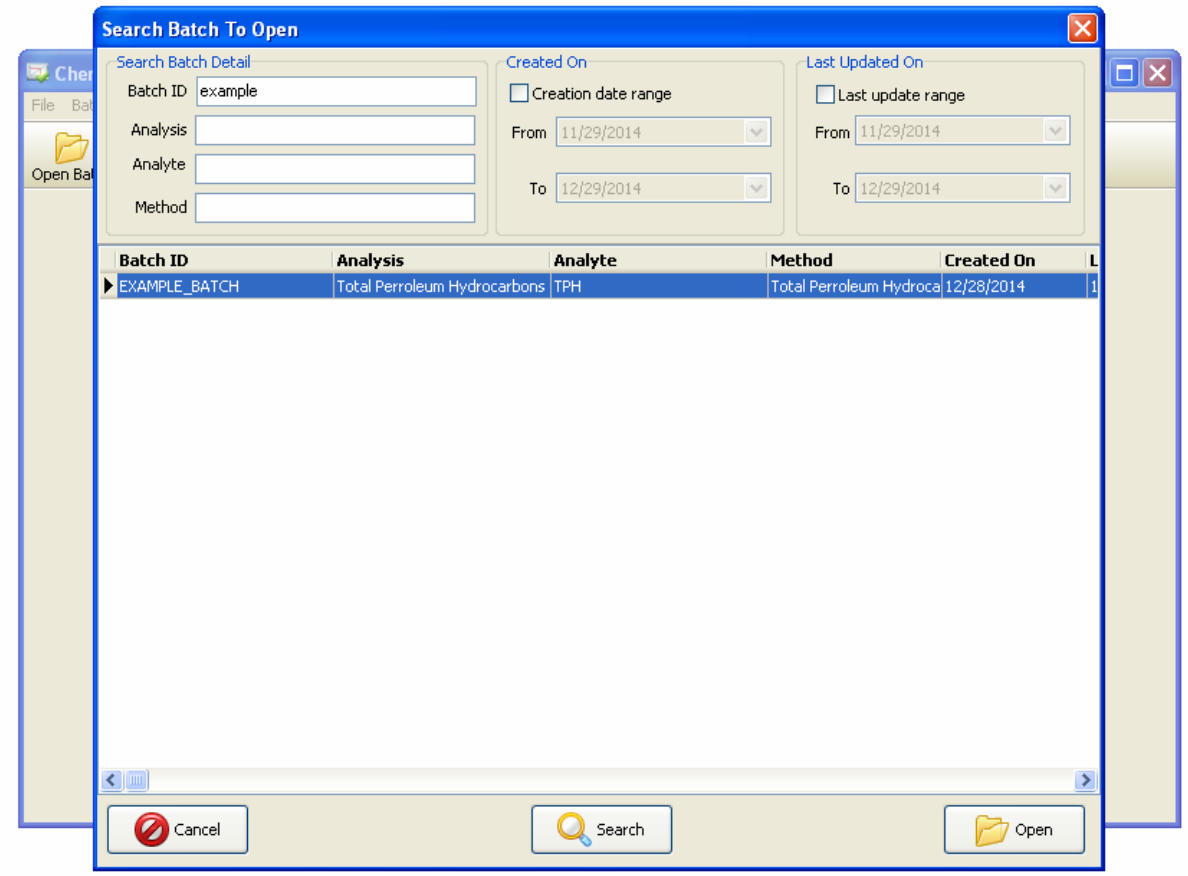
Format string 1234 and 0.5

Format string	1234	0.5
0	1234	1
0.00	1234.00	0.50
#.##	1234	.5
#,##0.00	1,234.00	0.50
#,##0.00	1,234.00	0.50

Note Tab
This tab is to enter user note for batch.

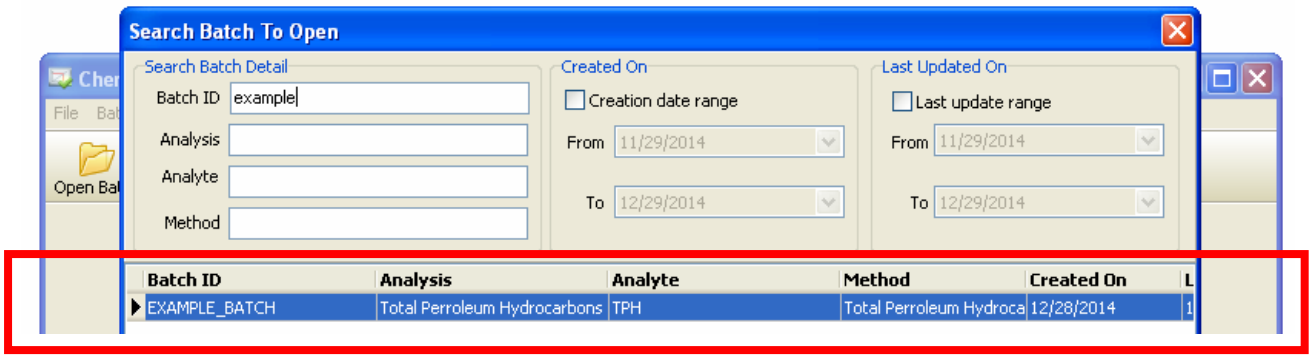
Open Existing Batch

To open existing batch, from toolbar click on **Open Batch** button. **Search Batch** dialog will show up. In **Search Batch** dialog, enter search conditions like (**Batch ID**, **Analysis** name or creation date…etc) and press **ENTER** or click **Search** button to see the result list. If search conditions have no result, message will appear. In the case you have to change search conditions.



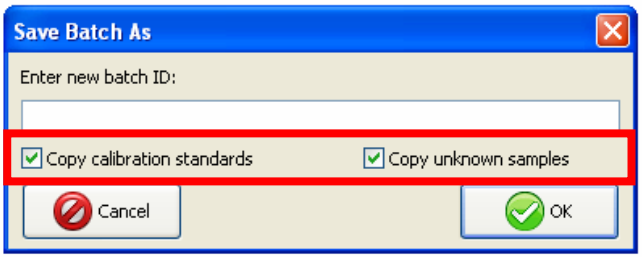
To list all batches available in the database, leave search fields empty and click **Search** button or press **ENTER**.

Click on column header to sort the result. Select batch you want and click **Open** button or press **ENTER**.

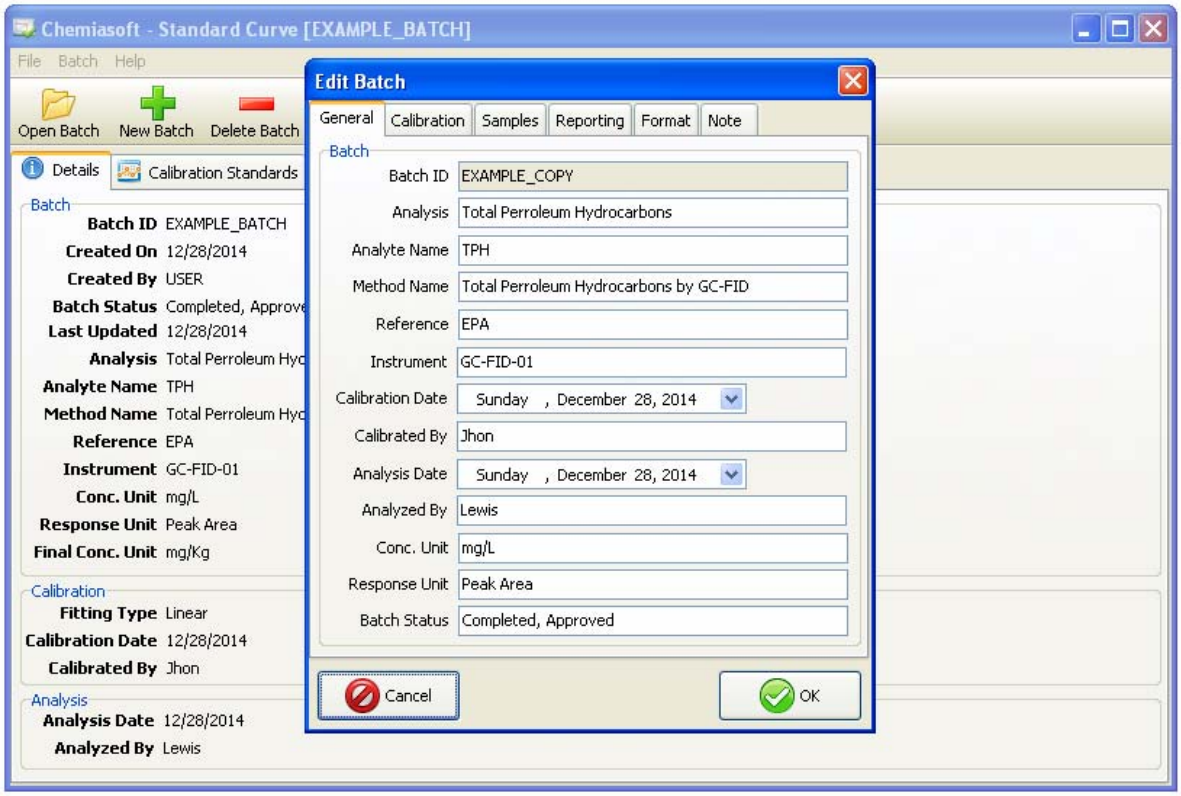


Save Batch As Different Name

Save batch as different name is similar to copy batch. First open the batch you want to copy and press **Save As** button. Save Batch As dialog will show up to enter new unique batch ID. Also, select if whether you want to copy calibration standards and samples to the new batch. There are two options with available at the bottom of the dialog (**Copy calibration standards** and **Copy unknown samples**).



Once you enter new batch ID, click **OK**. Then Edit Batch dialog will appear to make changes if there is any. Click **OK** or press **ENTER** when you are done.



Delete Existing Batch

To delete existing batch, open batch you want to delete. Click **Delete Batch** button from toolbar. A message will appear to confirm, click **Yes** to proceed.

Restore Deleted Batch

To restore deleted batch(s), go to menu **Batch** >> **Restore Deleted Batch**. **Restore Deleted Batch** dialog will show up. Select batch(s) you want to restore, then click **Restore Selection** to proceed.

Standards

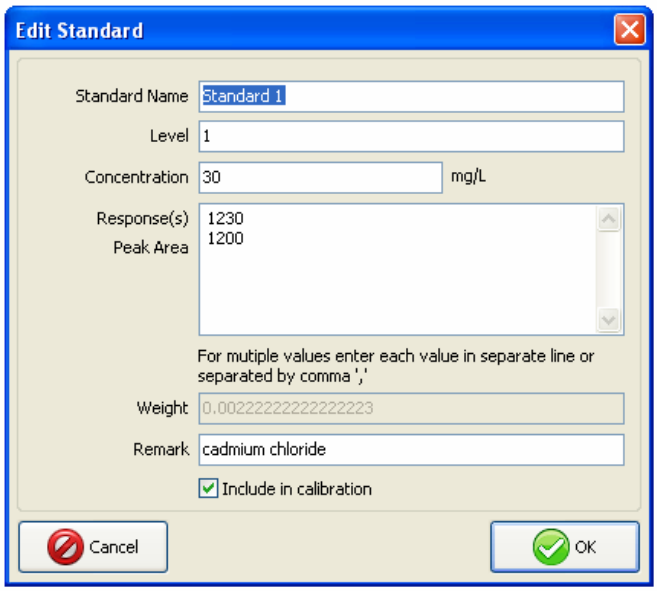
Add New Standard

To add new standard to batch click (**+**) button from standard table toolbar then **Edit Standard** dialog will show up.

Fill all information of the new standard. Below table explain each part:

Item	Description
Standard Name	Name of the standard (e.g. Standard One 25 ppm).
Number	Sequence order in the table. Standards are sorted in the table base on this number.
Concentration	Actual concentration of the analyte in the standard solution. Enter one value only.
Responses	Responses reading(s) from instruments used to run standard solution. You can enter single or multiple reading separated by comma. You may enter each ready in new line. The software will calculate the average and relative standard deviation RSD of the readings.
Weight	Weight factor required when weighted calibration is selected in **Batch Options**. There are manual and automatic calculations of weight.
Include in calibration points	Include or exclude standard from calibration curve.

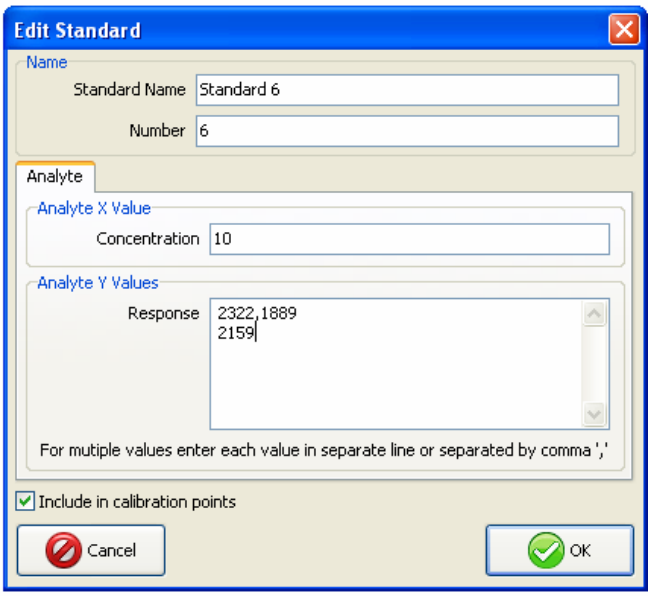
Click **OK** to proceed. Once you add new standard, the software will do recalibration and recalculate all samples.



Edit Existing Standard

To edit existing standard, **double click** standard you want to edit using left mouse button or select the standard using arrow up/down and press **ENTER**. Another way is to select standard and click on **Edit Standard** button from toolbar.

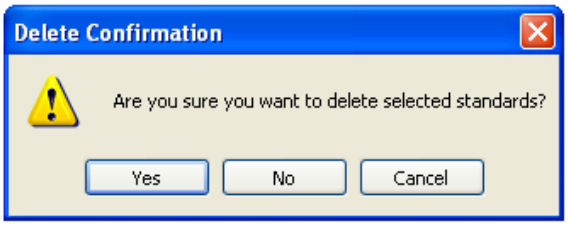
Edit Standard dialog will show up. Edit the standard information from the dialog and click **OK**. Once you edit standard, the software will do recalibration and recalculate all samples automatically.



Delete Existing Standard

To delete standard, select standard you want to delete by mouse or by using keyboard arrows up/down. Click (**-**) button from standard table toolbar.

From confirmation message, click **Yes** to proceed. Note that there is no undo for this step.



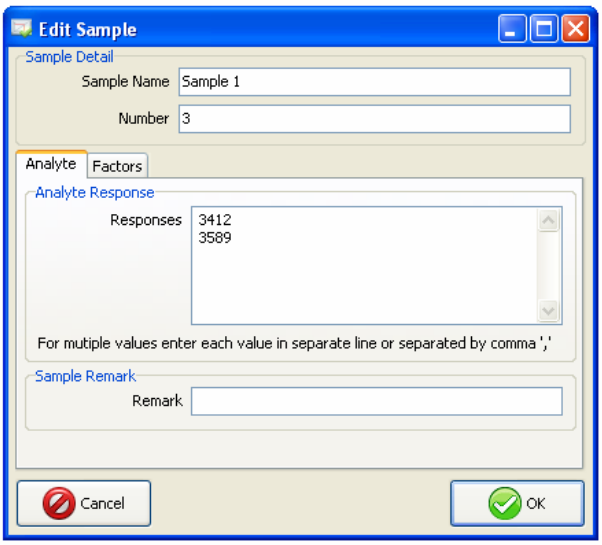
Recalibrate Batch Standards

When recalibrate batch, the software will do all calculations for fitting equation, will mTo recalibrate batch, from toolbar, click **Recalibrate Standards** button

Samples

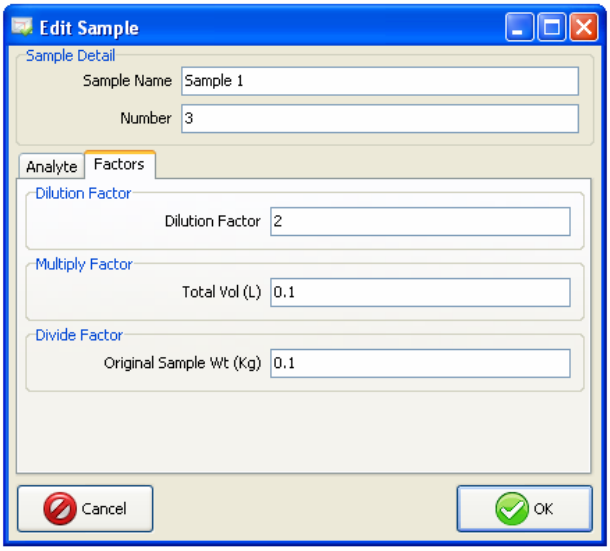
Add Sample to Batch

To add new sample to batch click (**+**) button from sample table toolbar then **Edit Sample** dialog will show up.



Fill all information of the new sample. Below table explain each part

Analyte Tab	
Item	**Description**
Sample Name	Name of the sample.
Number	Sequence order in the table. Samples are sorted in the table base on this number.
Responses	Responses reading(s) from instruments used to run sample solution. You can enter single or multiple reading separated by comma. You may enter each ready in new line. The software will calculate the average and relative standard deviation RSD of the readings.
Remarks	Note about the sample.

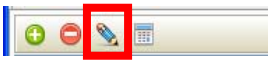


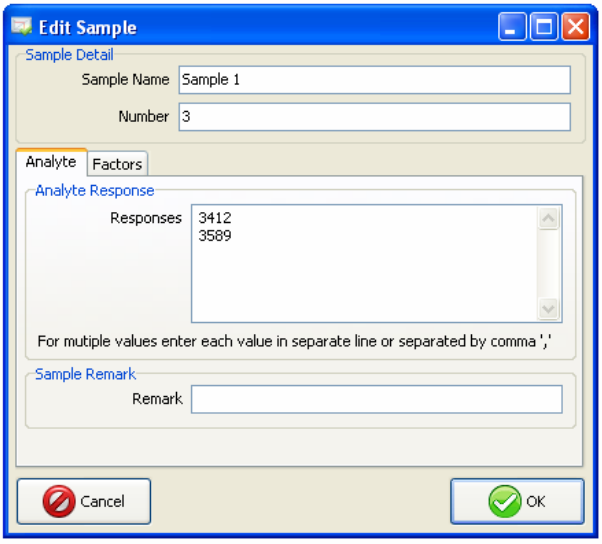
Factors Tab	
Item	**Description**
Dilution Factor	Dilution factors means how many times sample is diluted, more details about this factor in Edit Batch dialog. Calculated concentration from calibration equation will be multiplied by this factor. If the sample is not diluted then set this factor = 1
Multiply Factor	Usually its value is set to total sample solution volume in liter. This factor will multiply with calculated concentration from calibration equation. Factor name can be changed from Edit Batch dialog.
Divide Factor	Usually its value is set to initial sample weight in Kg. Calculated concentration from calibration equation will divide by this factor. Factor name can be changed from Edit Batch dialog.

Factors can be removed from Edit Batch dialog.

Edit Sample

To edit existing sample, **double click** sample you want to edit using left mouse button or select the sample using arrow up/down and press **ENTER**. Another way is to select sample and click on **Edit Sample** button from toolbar.



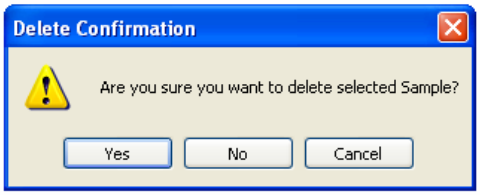


Edit Sample dialog will show up. Edit the sample information from the dialog and click **OK**. Once you edit standard, the software will do recalculate edited sample final concentration.

Delete sample

To delete sample, select sample you want to delete by mouse or by using keyboard arrows up/down. Click (**-**) button from sample toolbar.

From confirmation message, click **Yes** to proceed. Note that there is no undo for this step.



Recalculate Samples

When recalculate sample, the software will do all calculations for all samples, it will take responses and calculate concentrations base on calibration equation. From the toolbar, click **Recalculate Samples** button

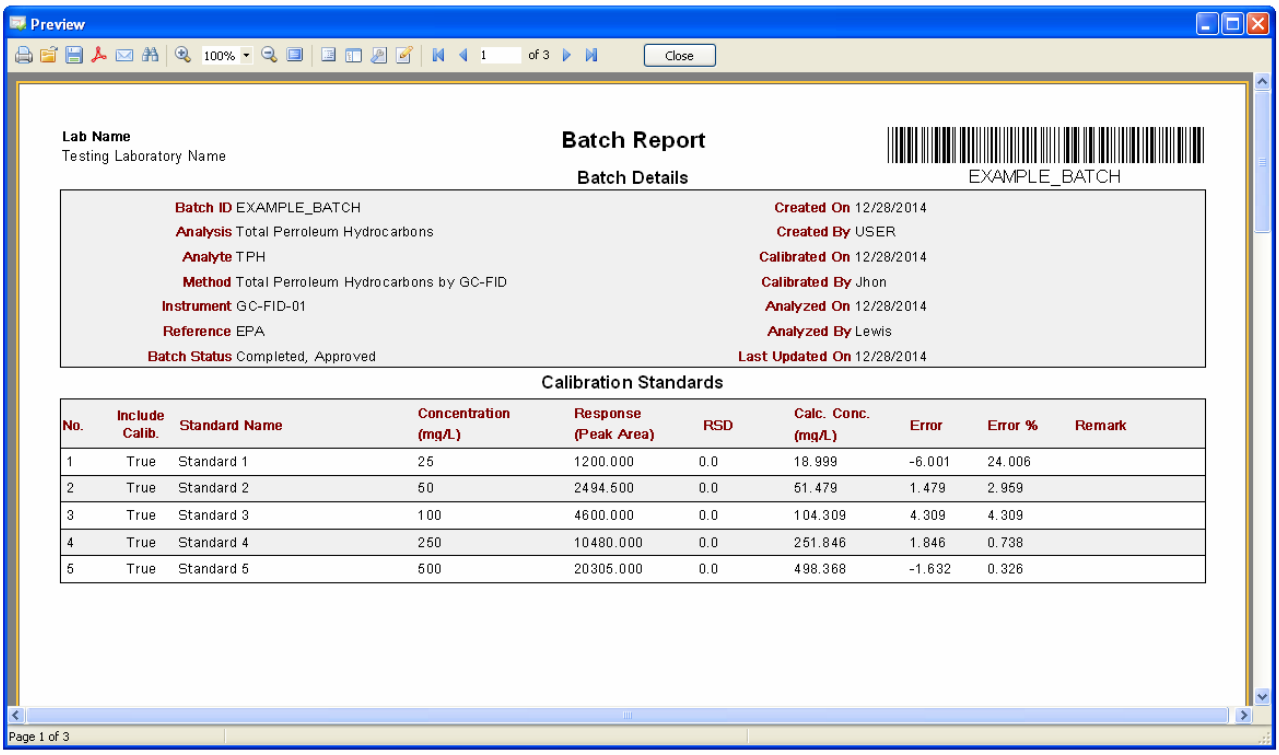
Note: This step will calculate all samples. It will **NOT** do recalibration of batch standards. If you want recalibration then see Recalibrate Batch.

Report

Batch report contains all batch details, standards and samples.

Generate Report

To generate batch report, open batch you want to report as per Open Existing Batch section. Click on Report button from toolbar, report will be generated on screen. Press **Print** button to print generated report.



Save Report

To save report from report screen click on **Save** button and select the format you want to save. You can save report in various formats (e.g. PDF, JPEG, PNG, MS Excel, MS Word … etc).

Registration

To register your copy **Standard Curve** do the following:

1. On **Standard Curve** software, go to menu **Help** >> **Registration**, the **Registration** dialog will show up.
2. Copy **Hardware ID**.
3. Visit www.chemiasoft.com and place your order for **Standard Curve**. Use the hardware ID while placing your order online, you will be asked for your hardware ID.
4. Once you complete your order, you will receive an email with the license information and registration code.
5. Copy the registration code from the email you received and paste it on the **Registration** dialog and click **Register** button. Welcome message will appear.
6. Close and restart **Standard Curve** to complete registration.
7. Enjoy using **Standard Curve** with full features.