The following is a sample calculation for Magnesium [MS-Excel 2013 is used]:

(1) Use your experimental data:

In MS-Excel, add your data and used the following formula to calculate: n, ΣX, ΣX^2 and D.

A	B	C	D	E	F	G
2	X = [Mg] ppm	Y = Abs.	X^2			
3	0.214	0.12	0.045796			
4	0.428	0.232	0.183184			
5	0.642	0.352	0.412164			
6	0.856	0.464	0.732736			
7	0.963	0.525	0.927369			
8						
9						
10	**Function:**	**Symbol**	**Value**			
11	COUNT(B3:B7)	n	5			
12	SUM(B3:B7)	SUM(X)	3.103	ΣX		
13	SUM(D3:D7)	SUM(X*X)	2.301249	ΣX^2		
14	(D11)(D13)-(D12)^2	D	1.877636			

Use: Tool>>Data Analysis>> Regression.

Choose: Input Y range, Input X range, Output range location for the output data.

	SUMMARY OUTPUT					
	Regression Statistics					
	Multiple R	0.999926693				
	R Square	**0.999853391**				
	Adjusted R Square	0.999804521				
	Standard Error	**0.002316431**				
	Observations	5				
	ANOVA					
		df	*SS*	*MS*	*F*	*Significance F*
	Regression	1	0.109783102	0.109783	20459.58	7.53E-07
	Residual	3	1.60976E-05	5.37E-06		
	Total	4	0.1097992			
		Coefficients	*Standard Error*	*t Stat*	*P-value*	
	Intercept	**0.00304878**	**0.002564458**	1.18886	0.320023	
	X Variable 1 (**Slope**)	**0.5406884**	**0.00378006**	143.037	7.53E-07	

(2) Organize your statistic data:

Based on the above output "*Regression Statistics*", you have the following data:

Slope:	*Coefficients*	**0.5406884**
Intercept:	*Coefficients*	**0.00304878**
S_m :	*Standard Error for Coefficients*	0.00378006
S_b	*Standard Error for Coefficients*	0.002564458
R^2		0.999853391
S_y	Standard Error	0.002316431

(3) Prepare your graph:

Choose: XY-Scatter.

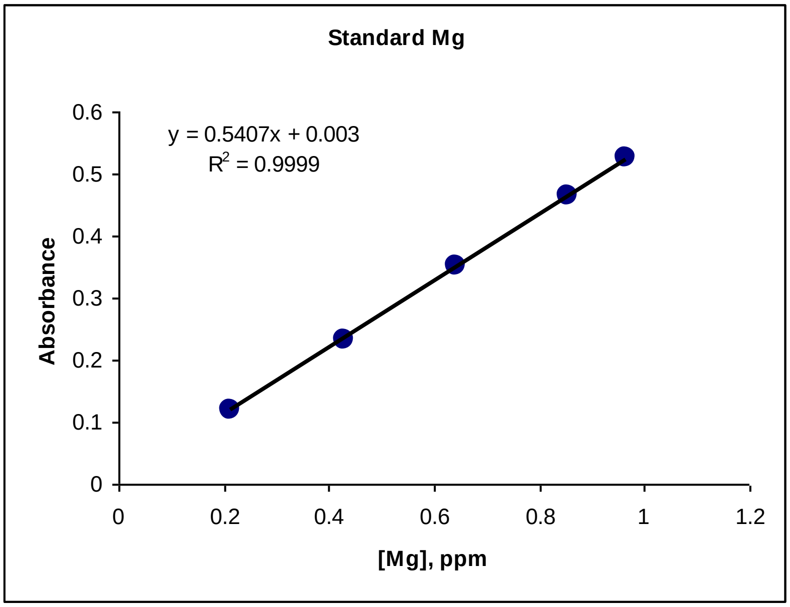
Choose: Sub-Type (Compares pairs of values). Data points without line!

On your graph click on the data-point (marker), choose "Add trend line".

Choose: Linear, (go to options), add check marks for:

Display equation on chart.

Display R-Squared value on chart.



(4) Calculate the concentration of diluted unknown, based on the Mg equation:

Abs = **0.5406884** [Mg] + **0.00304878**

Using Equation of the Line to find [Mg] in the Unknown Solution	
Absorbance	[Mg] ppm, calculated
0.198	0.361
0.253	**0.462**
0.292	0.534

(5) Calculate uncertainty in diluted unknown concentration:

$$\sigma_x = \frac{\sigma_y}{|m|}\sqrt{\left[\frac{1}{k}+\frac{1}{n}+\frac{(y-\bar{y})^2}{m^2\sum(x_i-\bar{x})^2}\right]}$$

σ_y = Standard Error
m = Slope = 0.5407
k = Number of replicate measurements
n = Number of data point = 5
y_i = Absorbance of standard solutions (i = 1, 2, 3, … 5)

x	y	**y** **cal** = (slope) X + (intercept)	d_i = y - **y**cal	$(d_i - \bar{d})^2$
0.214	0.120	0.11876	d_i = 0.120 - 0.11876 = 1.24 E-3	9.025E-7
0.428	0.232	0.2352	-3.20E-3	1.22E-5
0.642	0.352	0.35017	1.83E-3	2.372E-6
0.856	0.464	0.46661	-2.61E-3	8.41E-6
0.963	0.525	0.52373	1.28E-3	9.80E-7
[Mg] STD	**Recorded Abs.**	**Calculated Abs.**	**Average (d_i): $\bar{d}$ = -2.92 E-4**	**Total: 2.486E-5**

$$\sigma_y \approx S_y = \sqrt{\frac{1}{n-2}\sum\left(d_i - \bar{d}\right)^2} = \sqrt{\frac{2.486\times10^{-5}}{3}} = 2.878\times10^{-3}$$

$$\bar{y} = \frac{0.120+0.232+0.352+0.464+0.525}{5}\ 0.3386$$

$$\bar{x} = \frac{\sum x}{n} = \frac{3.103}{5} = 0.6206$$

$$\sum\left(x-\bar{x}\right)^2 = \left[(0.214-0.6206)^2+(0.428-0.6206)^2+(0.642-0.6206)^2+(0.856-0.6206)^2+(0.0.963-0.6206)^2\right]$$

$$\sum\left(x-\bar{x}\right)^2 = \left[(0.16532)+(0.03709)+(4.5796\times10^{-4})+(0.055413)+(0.117238)\right] = 0.37552$$

$$\sigma_x = \frac{0.0023164}{0.540688}\sqrt{\left[\frac{1}{1}+\frac{1}{5}+\frac{(y-\bar{y})^2}{m^2\sum(x_i-\bar{x})^2}\right]}$$

$$\sigma_x = \frac{0.002316}{0.5407}\sqrt{\left[1+(0.462)^2\left(\frac{5}{1.8776}\right)+\frac{2.3012}{1.8776}-2\,(0.462)\,\frac{3.103}{1.8776}\right]}$$

$$\sigma_x = 4.28\times10^{-3}\sqrt{[1+0.5684+1.2256-1.5270]}$$

$$\sigma_x = 4.28\times10^{-3} \times 1.1256 = 4.8175\times10^{-3}$$

(6) Use dilution factor (1:100) for the Mg-unknown solution the find the Original Solution Concentration:

Therefore, for the trial 2: $0.462\ ppm \times \frac{100}{1} = 46.2\ ppm$

(7) Uncertainty in original concentration:

$$\frac{\sigma_x(org)}{Conc.\ org} = \frac{\sigma_x(dil)}{Conc.\ dil}$$

$$\sigma_X = (Conc.\ Org)\times\frac{\sigma_x(dil)}{Conc.\ dil}$$

$$\sigma_X = (46.2\ ppm)\times\frac{4.8175\times10^{-3}}{0.462\ ppm} = 0.482$$

(8) Original Concentration of Mg ($\sigma_X = 0.5$):

$C_{[Mg]} \pm \sigma_X$ ppm

$$\boxed{46.2 \pm 0.5 \text{ ppm}}$$

Do same calculations in order for the Calcium and tap water!

Calculate total hardness, using your results of the AAS measurements:

$$[CaCO_3]_{ppm} = \frac{100.1\ g/_{mol}\ CaCO_3}{40.1 g/_{mol}\ Ca}\cdot[Ca^{2+}]^{AAS}_{ppm} + \frac{100.1\ g/_{mol}\ CaCO_3}{24.1 g/_{mol}\ Mg}\cdot[Mg^{2+}]^{AAS}_{ppm}$$

$$[CaCO_3]_{ppm} = 2.50\cdot[Ca^{2+}]^{AAS}_{ppm} + 4.12\cdot[Mg^{2+}]^{AAS}_{ppm}$$