

SPREADSHEET PROFICIENCY TEST

The purpose of this exercise is to be sure that you have the skills necessary to use a spreadsheet (Excel) for calculations and plotting of data. You should turn in this test by the date indicated in the class schedule. See the web page (link on CH 461 home page under Supplemental Materials) <http://www.chemistry.oregonstate.edu/courses/ch361-464/ch461/Spreadsheet461.htm> for information about spreadsheets. You can also get help on using Excel from the MS web page-just select the F1 key in Excel, and of course, ask your GTA's for assistance.

Feel free to get advice from a TA, faculty member, or friend. If you are having trouble, arrange to meet a TA or instructor at the end of the laboratory period. After you have mastered the necessary skills, you are to complete this test on your own and turn in your own spreadsheet and graph. Submitting any part of another student's spreadsheet defeats the purpose of the exercise and is not allowed.

The following spectrophotometric data has been obtained using a photodiode array spectrometer for the determination of vitamin D3 (cholecalciferol) in ethanol at a wavelength of 264 nm.

Transmittance	C/mM
0.191	1.561
0.244	1.333
0.378	0.917
0.502	0.650
0.647	0.411

Your task is to work up the calibration curve according to the following instructions and submit a hardcopy.

- Title** the spreadsheet (include your name and date in the title), and **start a data table** in the body of the spreadsheet and labeling four columns as C, T, A, and A', (concentration, transmittance, experimental measured absorbance, calculated absorbance from linear regression analysis (LR)), entering units in the top heading of the C column, and entering the data above into the C and T columns of the spreadsheet.
- Find the calculated absorbance from the measured transmittance** (recall that $A = -\log_{10}T$). Do this for each concentration in the A column of the spreadsheet by using the **copy command** to copy the formula you just entered for the first cell to all the other cells in that column (see point 9 on the web page on spreadsheets link above).
- Highlight columns A and C only, then on the top menu go to **"Insert - Scatter"** to enter the **graph wizard** to generate an x-y scatter plot of A vs C. Select the "markers only" display (do not connect the markers with a line). Add a graph title (which includes a descriptive title and your last name and the date). Add labels on the axes. Size the font so that it looks good. **Do not add a trendline** at this time. Select **Chart Tools** at the top of the screen for expanded menu for Chart.
- Run a **linear regression (LR) analysis** for **A vs C** (note: convention is **Y vs X**). Do this by selecting: **Data-Data Analysis- -Regression**. Do not choose "constant is zero" because this forces a zero intercept. The **Output** should be placed below the data table in the spreadsheet. If the Menu does not

have this option, choose Add-Ins (file-options-addins) first and select Regression, press enter. This will add the Data Analysis option to Data menu with Regression on the submenu.

5. Use the slope and intercept from the summary output table from LR to calculate the **expected values of A (this is A')** from the equation for a straight line using the slope and intercept reported from LR by copying and pasting the values for the slope and intercept from the summary table. Put the calculation for A' in the fourth column of your spreadsheet. Calculate the A' expected value for all concentrations in the table by copying the formula down the column.

6. In the third and fourth columns of the spreadsheet data table, arrange for the headings and numbers in the columns to be centered and for display of three significant figures (three places to right of decimal point). Even though absorbance is unitless, you can use "AU" to designate absorbance. Report the AU values to 1 mAU precision.

7. Adjust the chart so that the x-axis goes from 0 to 2.0 with a tick mark every 0.5 mM and the y-axis from -0.50 to 1.00 absorbance unit (AU) with a tick mark every 0.20 AU. The **data points should be plotted as markers only and A' values from LR fit plotted as a solid line only** that is forecasted back to the origin (0,0). Give a proper Name to each plotted series (e.g., do not leave as series 1 & 2). Most of these adjustments are found under **Format Axis**.

8. Annotate the graph with the equation of the line from LR in one textbox and provide the standard error (SE) of the slope and standard error (SE) of the intercept in another textbox. SE values are found in the LR summary output table to the right of the slope and intercept values, respectively. To add a textbox to a chart, select **Insert, Chart Tools, Text Box** at the top of the screen. To adjust the properties of the textbox, click on the textbox click the right mouse button for textbox menu. Set the Fill to white.

9. Check the list below. Compare your spreadsheet and graph to the sample that is attached. When you are satisfied, print your spreadsheet on one page - data table, summary table and graph. **Don't forget to put your name and the date on your copy.**

Additional Notes

This test is more than an exercise in that this test defines what we expect your spreadsheets to look like when you turn in your reports. Proper labeling, attention to significant figures, and reporting of the equation of the curve and standard errors are all part of a professional report.

Check your work for these corrections that are frequently needed

Correction	Occurrences in F 2018
clear default shaded background	10
add vertical grid lines	9
add standard error with labels	7
state equation as $A = x C + y$ (correct sf's)	7
make report fit on a single page	5
fix significant figures	5
transcribe SE data correctly to chart	5
align headings and data	4
use correct numbers for regression (C,A)	3
add horizontal grid lines	2
make title informative (beyond x vs y)	2
correct A' values	2
plot A' data	2
don't include R^2	2
delete excessive tics	2
make axes intersect at 0,0	1
remove extra data points in graph	1
make data point symbols easily visible	1
remove extraneous data from chart	1
use data from this year	1
make text box large enough to hold text	1
label data appropriately	1

Sample - Spectrophotometric Calibration for Vitamin C -- 9/25/18 THIS IS NOT THE DATA for 2019 and the axes ranges are different.!

C / mM	T	A	A'
0.00	1.000	0.000	0.000
1.00	0.785	0.105	0.097
3.00	0.524	0.281	0.291
10.0	0.107	0.971	0.968

SUMMARY OUTPUT

<i>Regression Statistics</i>	
Multiple R	0.999850896
R Square	0.999701813
Adjusted R Square	0.99955272
Standard Error	0.009234448
Observations	4

ANOVA					
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	0.571787015	0.571787015	6705.211	0.000149104
Residual	2	0.00017055	8.5275E-05		
Total	3	0.571957565			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	0.000243847	0.006200295	0.039328356	0.972201	-0.02643387	0.0269216	-0.026433869	0.02692156
C / mM Slope	0.096817135	0.00118235	81.88535154	0.000149	0.091729894	0.1019044	0.091729894	0.10190438

