# Comparison of Calibration Curve Fitting Methods in Absorption Spectroscopy

| Wavelength, nm | Spectral bandpass, nm | Absorber width, nm | Absorptivity ( x 10 ) | Absorption Path length | Unabsorbed stray light | Maximum concentration | Random Noise |
|---|---|---|---|---|---|---|---|
| 500 | 100 | 100 | 4 | 1 | =0.0001*A | 10 | ☐ Photon FALSE<br>☐ Detector FALSE |

**Click the arrows above to change the values**

5

**σ of errors** **=STDEV($Sheet2.E50:N50)**

Concentration=(A-intercept)/slope
where A = measured absorbance;
slope and intercept from first-order fit
of Absorbance vs Concentration.
slope= =slope

**σ of errors** **=STDEV(Sheet2.E60:N60)**

Concentration=(-b²+SQRT(b-4*a*(c-A)))/(2*a)
where A = measured absorbance;
a, b, and c = coefficients from quadratic fit
of Absorbance vs Concentration.
a= =aa

intercept= =intercept

b= =bb
c= =cc

| Named variables | |
|---|---|
| amax | Maximum absorptivity |
| aw | Absorber width (half-width of the absorption band) |
| b | Absorption path length |
| Izero | Incident intensity |
| sl | Stray light (fraction of incident light) |
| sw | Source width (spectral bandpass of monochromator) |
| slope | Slope of straight-line least squares fit to calibration curve |
| intercept | Intercept of straight-line least squares fit to calibration curve |
| W | Wavelength |
| aa,bb,cc | Coefficients of quadratic fit (avoids collison with b=path length |

Mininum C
0

| Concentration |
|---|
| =MinC |
| =H41+(MaxC-MinC)/9 |
| =H42+(MaxC-MinC)/9 |
| =H43+(MaxC-MinC)/9 |
| =H44+(MaxC-MinC)/9 |
| =H45+(MaxC-MinC)/9 |
| =H46+(MaxC-MinC)/9 |
| =H47+(MaxC-MinC)/9 |
| =H48+(MaxC-MinC)/9 |
| =H49+(MaxC-MinC)/9 |

99

Absorption peak shape

- (●) Gaussian
- ( ) Lorentzian

**σ of errors** **=STDEV($Sheet2.E76:N76)**

Concentration=a*A$^3$+b*A$^2$+c*A+d
where A = measured absorbance;
a, b, c, and d from reversed cubit fit
of reversed data (Concentration vs Absorbance).

a= =$Sheet2.E73

b= =$Sheet2.F73
c= =$Sheet2.G73
d= =$Sheet2.H73

| Absorbance |
|---|
| =$Sheet2.E46 |
| =$Sheet2.F46 |
| =$Sheet2.G46 |
| =$Sheet2.H46 |
| =$Sheet2.I46 |
| =$Sheet2.J46 |
| =$Sheet2.K46 |
| =$Sheet2.L46 |
| =$Sheet2.M46 |
| =$Sheet2.N46 |

| Wavelength | | Slit function |
|---|---|---|
| 400 | =1-200*ABS((A3-W)/(100))/(2*sw) | =sw*IF(B3<0;0;B3) |
| =A3+5 | =1-200*ABS((A4-W)/(100))/(2*sw) | =sw*IF(B4<0;0;B4) |
| =A4+5 | =1-200*ABS((A5-W)/(100))/(2*sw) | =sw*IF(B5<0;0;B5) |
| =A5+5 | =1-200*ABS((A6-W)/(100))/(2*sw) | =sw*IF(B6<0;0;B6) |
| =A6+5 | =1-200*ABS((A7-W)/(100))/(2*sw) | =sw*IF(B7<0;0;B7) |
| =A7+5 | =1-200*ABS((A8-W)/(100))/(2*sw) | =sw*IF(B8<0;0;B8) |
| =A8+5 | =1-200*ABS((A9-W)/(100))/(2*sw) | =sw*IF(B9<0;0;B9) |
| =A9+5 | =1-200*ABS((A10-W)/(100))/(2*sw) | =sw*IF(B10<0;0;B10) |
| =A10+5 | =1-200*ABS((A11-W)/(100))/(2*sw) | =sw*IF(B11<0;0;B11) |
| =A11+5 | =1-200*ABS((A12-W)/(100))/(2*sw) | =sw*IF(B12<0;0;B12) |
| =A12+5 | =1-200*ABS((A13-W)/(100))/(2*sw) | =sw*IF(B13<0;0;B13) |
| =A13+5 | =1-200*ABS((A14-W)/(100))/(2*sw) | =sw*IF(B14<0;0;B14) |
| =A14+5 | =1-200*ABS((A15-W)/(100))/(2*sw) | =sw*IF(B15<0;0;B15) |
| =A15+5 | =1-200*ABS((A16-W)/(100))/(2*sw) | =sw*IF(B16<0;0;B16) |
| =A16+5 | =1-200*ABS((A17-W)/(100))/(2*sw) | =sw*IF(B17<0;0;B17) |
| =A17+5 | =1-200*ABS((A18-W)/(100))/(2*sw) | =sw*IF(B18<0;0;B18) |
| =A18+5 | =1-200*ABS((A19-W)/(100))/(2*sw) | =sw*IF(B19<0;0;B19) |
| =A19+5 | =1-200*ABS((A20-W)/(100))/(2*sw) | =sw*IF(B20<0;0;B20) |
| =A20+5 | =1-200*ABS((A21-W)/(100))/(2*sw) | =sw*IF(B21<0;0;B21) |
| =A21+5 | =1-200*ABS((A22-W)/(100))/(2*sw) | =sw*IF(B22<0;0;B22) |
| =A22+5 | =1-200*ABS((A23-W)/(100))/(2*sw) | =sw*IF(B23<0;0;B23) |
| =A23+5 | =1-200*ABS((A24-W)/(100))/(2*sw) | =sw*IF(B24<0;0;B24) |
| =A24+5 | =1-200*ABS((A25-W)/(100))/(2*sw) | =sw*IF(B25<0;0;B25) |
| =A25+5 | =1-200*ABS((A26-W)/(100))/(2*sw) | =sw*IF(B26<0;0;B26) |
| =A26+5 | =1-200*ABS((A27-W)/(100))/(2*sw) | =sw*IF(B27<0;0;B27) |
| =A27+5 | =1-200*ABS((A28-W)/(100))/(2*sw) | =sw*IF(B28<0;0;B28) |
| =A28+5 | =1-200*ABS((A29-W)/(100))/(2*sw) | =sw*IF(B29<0;0;B29) |
| =A29+5 | =1-200*ABS((A30-W)/(100))/(2*sw) | =sw*IF(B30<0;0;B30) |
| =A30+5 | =1-200*ABS((A31-W)/(100))/(2*sw) | =sw*IF(B31<0;0;B31) |
| =A31+5 | =1-200*ABS((A32-W)/(100))/(2*sw) | =sw*IF(B32<0;0;B32) |
| =A32+5 | =1-200*ABS((A33-W)/(100))/(2*sw) | =sw*IF(B33<0;0;B33) |
| =A33+5 | =1-200*ABS((A34-W)/(100))/(2*sw) | =sw*IF(B34<0;0;B34) |
| =A34+5 | =1-200*ABS((A35-W)/(100))/(2*sw) | =sw*IF(B35<0;0;B35) |
| =A35+5 | =1-200*ABS((A36-W)/(100))/(2*sw) | =sw*IF(B36<0;0;B36) |
| =A36+5 | =1-200*ABS((A37-W)/(100))/(2*sw) | =sw*IF(B37<0;0;B37) |

| | | |
|---|---|---|
| =A37+5 | =1-200*ABS((A38-W)/(100))/(2*sw) | =sw*IF(B38<0;0;B38) |
| =A38+5 | =1-200*ABS((A39-W)/(100))/(2*sw) | =sw*IF(B39<0;0;B39) |
| =A39+5 | =1-200*ABS((A40-W)/(100))/(2*sw) | =sw*IF(B40<0;0;B40) |
| =A40+5 | =1-200*ABS((A41-W)/(100))/(2*sw) | =sw*IF(B41<0;0;B41) |
| =A41+5 | =1-200*ABS((A42-W)/(100))/(2*sw) | =sw*IF(B42<0;0;B42) |
| =A42+5 | =1-200*ABS((A43-W)/(100))/(2*sw) | =sw*IF(B43<0;0;B43) |
| | | Izero |
| Total intensity | | =SUM(C3:C43)*(1+sl) |
| Measured absorbance (y) | | |
| Theoretical absorbance | | |

Polynomial fits are computed by multilinear regression using the LINEST array function.
(Fit coefficients are displayed in red)

**Noise calculations**

Photon Noise

Detector noise

| Absorptivity |
| --- |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A3-500)/(0.5*aw))^2));amax/10*EXP(-1*((A3-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A4-500)/(0.5*aw))^2));amax/10*EXP(-1*((A4-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A5-500)/(0.5*aw))^2));amax/10*EXP(-1*((A5-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A6-500)/(0.5*aw))^2));amax/10*EXP(-1*((A6-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A7-500)/(0.5*aw))^2));amax/10*EXP(-1*((A7-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A8-500)/(0.5*aw))^2));amax/10*EXP(-1*((A8-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A9-500)/(0.5*aw))^2));amax/10*EXP(-1*((A9-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A10-500)/(0.5*aw))^2));amax/10*EXP(-1*((A10-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A11-500)/(0.5*aw))^2));amax/10*EXP(-1*((A11-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A12-500)/(0.5*aw))^2));amax/10*EXP(-1*((A12-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A13-500)/(0.5*aw))^2));amax/10*EXP(-1*((A13-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A14-500)/(0.5*aw))^2));amax/10*EXP(-1*((A14-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A15-500)/(0.5*aw))^2));amax/10*EXP(-1*((A15-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A16-500)/(0.5*aw))^2));amax/10*EXP(-1*((A16-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A17-500)/(0.5*aw))^2));amax/10*EXP(-1*((A17-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A18-500)/(0.5*aw))^2));amax/10*EXP(-1*((A18-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A19-500)/(0.5*aw))^2));amax/10*EXP(-1*((A19-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A20-500)/(0.5*aw))^2));amax/10*EXP(-1*((A20-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A21-500)/(0.5*aw))^2));amax/10*EXP(-1*((A21-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A22-500)/(0.5*aw))^2));amax/10*EXP(-1*((A22-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A23-500)/(0.5*aw))^2));amax/10*EXP(-1*((A23-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A24-500)/(0.5*aw))^2));amax/10*EXP(-1*((A24-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A25-500)/(0.5*aw))^2));amax/10*EXP(-1*((A25-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A26-500)/(0.5*aw))^2));amax/10*EXP(-1*((A26-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A27-500)/(0.5*aw))^2));amax/10*EXP(-1*((A27-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A28-500)/(0.5*aw))^2));amax/10*EXP(-1*((A28-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A29-500)/(0.5*aw))^2));amax/10*EXP(-1*((A29-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A30-500)/(0.5*aw))^2));amax/10*EXP(-1*((A30-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A31-500)/(0.5*aw))^2));amax/10*EXP(-1*((A31-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A32-500)/(0.5*aw))^2));amax/10*EXP(-1*((A32-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A33-500)/(0.5*aw))^2));amax/10*EXP(-1*((A33-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A34-500)/(0.5*aw))^2));amax/10*EXP(-1*((A34-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A35-500)/(0.5*aw))^2));amax/10*EXP(-1*((A35-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A36-500)/(0.5*aw))^2));amax/10*EXP(-1*((A36-500)/(0.6006*aw))^2)) |
| =IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A37-500)/(0.5*aw))^2));amax/10*EXP(-1*((A37-500)/(0.6006*aw))^2)) |

```
=IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A38-500)/(0.5*aw))^2));amax/10*EXP(-1*((A38-500)/(0.6006*aw))^2))
=IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A39-500)/(0.5*aw))^2));amax/10*EXP(-1*((A39-500)/(0.6006*aw))^2))
=IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A40-500)/(0.5*aw))^2));amax/10*EXP(-1*((A40-500)/(0.6006*aw))^2))
=IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A41-500)/(0.5*aw))^2));amax/10*EXP(-1*((A41-500)/(0.6006*aw))^2))
=IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A42-500)/(0.5*aw))^2));amax/10*EXP(-1*((A42-500)/(0.6006*aw))^2))
=IF($Sheet1.$I$3="FALSE";amax/10*(1/(1+((A43-500)/(0.5*aw))^2));amax/10*EXP(-1*((A43-500)/(0.6006*aw))^2))
```

Total transmitted intensity

Measured absorbance A =

amax*b*c=

**Linear Fit** Predicted concentration =

Concentration error (real-predicted)

Concentration error as % of max concentration

Straight-line fit computed via slope and intercept functions =>

**Quadratic Fit (absorbance vs concentration)**

C

$C^2$

Multilinear regression LINEST(Ameas;E55:N56;0;0)

predicted concentration (using the Quadratic Formula)

error

relative error as percentage of maximum

**Reversed quadratic fit (concentration vs absorbance)**

A

$A^2$

LINEST(concentrations;E63:N64;0;0) =>

predicted concentration

error

relative error as percentage of maximum

**Reversed cubic fit (concentration vs absorbance)**

A

$A^2$

$A^3$

LINEST(concentrations;E70:N72;0;0) =>

predicted concentration
error
relative error as percentage of maximum

**Random Noise calculations**

Photon noise
=SQRT(Izero)/2000

Detector noise
1.00E-03

| =$Sheet1.H41 | =$Sheet1.H42 |
|---|---|
| =$C3*10^(-$D3*b*E$2) | =$C3*10^(-$D3*b*F$2) |
| =$C4*10^(-$D4*b*E$2) | =$C4*10^(-$D4*b*F$2) |
| =$C5*10^(-$D5*b*E$2) | =$C5*10^(-$D5*b*F$2) |
| =$C6*10^(-$D6*b*E$2) | =$C6*10^(-$D6*b*F$2) |
| =$C7*10^(-$D7*b*E$2) | =$C7*10^(-$D7*b*F$2) |
| =$C8*10^(-$D8*b*E$2) | =$C8*10^(-$D8*b*F$2) |
| =$C9*10^(-$D9*b*E$2) | =$C9*10^(-$D9*b*F$2) |
| =$C10*10^(-$D10*b*E$2) | =$C10*10^(-$D10*b*F$2) |
| =$C11*10^(-$D11*b*E$2) | =$C11*10^(-$D11*b*F$2) |
| =$C12*10^(-$D12*b*E$2) | =$C12*10^(-$D12*b*F$2) |
| =$C13*10^(-$D13*b*E$2) | =$C13*10^(-$D13*b*F$2) |
| =$C14*10^(-$D14*b*E$2) | =$C14*10^(-$D14*b*F$2) |
| =$C15*10^(-$D15*b*E$2) | =$C15*10^(-$D15*b*F$2) |
| =$C16*10^(-$D16*b*E$2) | =$C16*10^(-$D16*b*F$2) |
| =$C17*10^(-$D17*b*E$2) | =$C17*10^(-$D17*b*F$2) |
| =$C18*10^(-$D18*b*E$2) | =$C18*10^(-$D18*b*F$2) |
| =$C19*10^(-$D19*b*E$2) | =$C19*10^(-$D19*b*F$2) |
| =$C20*10^(-$D20*b*E$2) | =$C20*10^(-$D20*b*F$2) |
| =$C21*10^(-$D21*b*E$2) | =$C21*10^(-$D21*b*F$2) |
| =$C22*10^(-$D22*b*E$2) | =$C22*10^(-$D22*b*F$2) |
| =$C23*10^(-$D23*b*E$2) | =$C23*10^(-$D23*b*F$2) |
| =$C24*10^(-$D24*b*E$2) | =$C24*10^(-$D24*b*F$2) |
| =$C25*10^(-$D25*b*E$2) | =$C25*10^(-$D25*b*F$2) |
| =$C26*10^(-$D26*b*E$2) | =$C26*10^(-$D26*b*F$2) |
| =$C27*10^(-$D27*b*E$2) | =$C27*10^(-$D27*b*F$2) |
| =$C28*10^(-$D28*b*E$2) | =$C28*10^(-$D28*b*F$2) |
| =$C29*10^(-$D29*b*E$2) | =$C29*10^(-$D29*b*F$2) |
| =$C30*10^(-$D30*b*E$2) | =$C30*10^(-$D30*b*F$2) |
| =$C31*10^(-$D31*b*E$2) | =$C31*10^(-$D31*b*F$2) |
| =$C32*10^(-$D32*b*E$2) | =$C32*10^(-$D32*b*F$2) |
| =$C33*10^(-$D33*b*E$2) | =$C33*10^(-$D33*b*F$2) |
| =$C34*10^(-$D34*b*E$2) | =$C34*10^(-$D34*b*F$2) |
| =$C35*10^(-$D35*b*E$2) | =$C35*10^(-$D35*b*F$2) |
| =$C36*10^(-$D36*b*E$2) | =$C36*10^(-$D36*b*F$2) |
| =$C37*10^(-$D37*b*E$2) | =$C37*10^(-$D37*b*F$2) |

| | |
|---|---|
| =$C38*10^(-$D38*b*E$2) | =$C38*10^(-$D38*b*F$2) |
| =$C39*10^(-$D39*b*E$2) | =$C39*10^(-$D39*b*F$2) |
| =$C40*10^(-$D40*b*E$2) | =$C40*10^(-$D40*b*F$2) |
| =$C41*10^(-$D41*b*E$2) | =$C41*10^(-$D41*b*F$2) |
| =$C42*10^(-$D42*b*E$2) | =$C42*10^(-$D42*b*F$2) |
| =$C43*10^(-$D43*b*E$2) | =$C43*10^(-$D43*b*F$2) |
| | |
| =SUM(E3:E43)+sl*$C$45 | =SUM(F3:F43)+sl*$C$45 |
| =LOG(ABS((Izero+E78+E82)/(E45+E79+E83));10) | =LOG(ABS((Izero+F78+F82)/(F45+F79+F83));10) |
| =E2*$D$23*b | =F2*$D$23*b |
| =(E46-intercept)/slope | =(F46-intercept)/slope |
| =E2-E48 | =F2-F48 |
| =E49/MAX($E$2:$N$2) | =F49/MAX($E$2:$N$2) |
| | slope= |
| | Intercept= |
| | R2= |
| | |
| =E2 | =F2 |
| =E55^2 | =F55^2 |
| {=LINEST(Ameas;E55:N56;0;0)} | {=LINEST(Ameas;E55:N56;0;0)} |
| =(-bb+SQRT(bb*bb-4*aa*(cc-E46)))/(2*aa) | =(-bb+SQRT(bb*bb-4*aa*(cc-F46)))/(2*aa) |
| =E58-E2 | =F58-F2 |
| =E59/MAX($E$2:$N$2) | =F59/MAX($E$2:$N$2) |
| | |
| | |
| =E46 | =F46 |
| =E63^2 | =F63^2 |
| {=LINEST(concentrations;E63:N64;0;0)} | {=LINEST(concentrations;E63:N64;0;0)} |
| =$E$65*E64+$F$65*E63+$G$65 | =$E$65*F64+$F$65*F63+$G$65 |
| =E66-E2 | =F66-F2 |
| =E67/MAX($E$2:$N$2) | =F67/MAX($E$2:$N$2) |
| | |
| =E63 | =F63 |
| =E70^2 | =F70^2 |
| =E70^3 | =F70^3 |
| {=LINEST(concentrations;E70:N72;0;0)} | {=LINEST(concentrations;E70:N72;0;0)} |

| | |
|---|---|
| =$E$73*E72+$F$73*E71+$G$73*E70+$H$73 | =$E$73*F72+$F$73*F71+$G$73*F70+$H$73 |
| =E74-E2 | =F74-F2 |
| =E75/MAX($E$2:$N$2) | =F75/MAX($E$2:$N$2) |

Photon noise in Izero and I, respectively (if “Photo” is checked under “Random Noise”)

| | |
|---|---|
| =IF($Sheet1.$H$3="TRUE";$D$79*(2.5*(RAND()-RAND()));0) | =IF($Sheet1.$H$3="TRUE";$D$79*(2.5*(RAND()-RAND()));0) |
| =IF($Sheet1.$H$3="TRUE";SQRT(E45)*(2.5*(RAND()-RAND())/1000);0) | ### |

Detector noise in Izero and I, respectively (if “Detector” is checked under “Random Noise”)

| | |
|---|---|
| =IF($Sheet1.$H$4="TRUE";$D$82*(2.5*(RAND()-RAND()));0) | =IF($Sheet1.$H$4="TRUE";$D$82*(2.5*(RAND()-RAND()));0) |
| =IF($Sheet1.$H$4="TRUE";$D$82*(2.5*(RAND()-RAND()));0) | =IF($Sheet1.$H$4="TRUE";$D$82*(2.5*(RAND()-RAND()));0) |

| Concentration | | | | | | | |
|---|---|---|---|---|---|---|---|
| =$Sheet1.H43 | ### | ### | ### | ### | ### | ### | ### |
| =$C3*10^(-$D3*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C4*10^(-$D4*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C5*10^(-$D5*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C6*10^(-$D6*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C7*10^(-$D7*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C8*10^(-$D8*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C9*10^(-$D9*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C10*10^(-$D10*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C11*10^(-$D11*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C12*10^(-$D12*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C13*10^(-$D13*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C14*10^(-$D14*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C15*10^(-$D15*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C16*10^(-$D16*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C17*10^(-$D17*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C18*10^(-$D18*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C19*10^(-$D19*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C20*10^(-$D20*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C21*10^(-$D21*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C22*10^(-$D22*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C23*10^(-$D23*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C24*10^(-$D24*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C25*10^(-$D25*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C26*10^(-$D26*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C27*10^(-$D27*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C28*10^(-$D28*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C29*10^(-$D29*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C30*10^(-$D30*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C31*10^(-$D31*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C32*10^(-$D32*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C33*10^(-$D33*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C34*10^(-$D34*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C35*10^(-$D35*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C36*10^(-$D36*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C37*10^(-$D37*b*G$2) | ### | ### | ### | ### | ### | ### | ### |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| =$C38*10^(-$D38*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C39*10^(-$D39*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C40*10^(-$D40*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C41*10^(-$D41*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C42*10^(-$D42*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| =$C43*10^(-$D43*b*G$2) | ### | ### | ### | ### | ### | ### | ### |
| | | | | | | | |
| =SUM(G3:G43)+sl*$C$45 | ### | ### | ### | ### | ### | ### | ### |
| ### | ### | ### | ### | ### | ### | ### | ### |
| =G2*$D$23*b | ### | ### | ### | ### | ### | ### | ### |
| =(G46-intercept)/slope | ### | ### | ### | ### | ### | ### | ### |
| =G2-G48 | =H2-H48 | =I2-I48 | =J2-J48 | =K2-K48 | =L2-L48 | =M2-M48 | =N2-N48 |
| =G49/MAX($E$2:$N$2) | ### | ### | ### | ### | ### | ### | ### |
| =SLOPE(E$46:N$46;E$2:N$2) | | | | | | | |
| =INTERCEPT(E$46:N$46;E$2:N$2) | | | | | | | |
| =RSQ(E$46:N$46;E$47:N$47) | | | | | | | |
| | | | | | | | |
| =G2 | =H2 | =I2 | =J2 | =K2 | =L2 | =M2 | =N2 |
| =G55^2 | =H55^2 | =I55^2 | =J55^2 | =K55^2 | =L55^2 | =M55^2 | =N55^2 |
| {=LINEST(Ameas;E55:N56;0;0)} | | | | | | | |
| =(-bb+SQRT(bb*bb-4*aa*(cc-G46)))/(2*aa) | ### | ### | ### | ### | ### | ### | ### |
| =G58-G2 | =H58-H2 | =I58-I2 | =J58-J2 | =K58-K2 | =L58-L2 | =M58-M2 | =N58-N2 |
| =G59/MAX($E$2:$N$2) | ### | ### | ### | ### | ### | ### | ### |
| | | | | | | | |
| =G46 | =H46 | =I46 | =J46 | =K46 | =L46 | =M46 | =N46 |
| =G63^2 | =H63^2 | =I63^2 | =J63^2 | =K63^2 | =L63^2 | =M63^2 | =N63^2 |
| {=LINEST(concentrations;E63:N64;0;0)} | | | | | | | |
| =$E$65*G64+$F$65*G63+$G$65 | ### | ### | ### | ### | ### | ### | ### |
| =G66-G2 | =H66-H2 | =I66-I2 | =J66-J2 | =K66-K2 | =L66-L2 | =M66-M2 | =N66-N2 |
| =G67/MAX($E$2:$N$2) | ### | ### | ### | ### | ### | ### | ### |
| | | | | | | | |
| =G63 | =H63 | =I63 | =J63 | =K63 | =L63 | =M63 | =N63 |
| =G70^2 | =H70^2 | =I70^2 | =J70^2 | =K70^2 | =L70^2 | =M70^2 | =N70^2 |
| =G70^3 | =H70^3 | =I70^3 | =J70^3 | =K70^3 | =L70^3 | =M70^3 | =N70^3 |
| {=LINEST(concentrations;E70:N72;0;0)} | ### | | | | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| ### | ### | ### | ### | ### | ### | ### | ### |
| =G74-G2 | =H74-H2 | =I74-I2 | =J74-J2 | =K74-K2 | =L74-L2 | =M74-M2 | =N74-N2 |
| =G75/MAX($E$2:$N$2) | ### | ### | ### | ### | ### | ### | ### |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| ### | ### | ### | ### | ### | ### | ### | ### |
| ### | ### | ### | ### | ### | ### | ### | ### |
| | | | | | | | |
| ### | ### | ### | ### | ### | ### | ### | ### |
| ### | ### | ### | ### | ### | ### | ### | ### |

Introduction

The purpose of this simulation is to compare three methods of least-squa
spectrophotometry calibration curves with varying degrees of non-lineari
unabsorbed stray light (see Background information, below). The operat
from Beer's Law"; it computes the measured absorbance and plots the a
concentration) for a simulated series of simulated absorber concentration
spectrophotometer with variable spectral bandpass and unabsorbed stray
path length, half-width of the absorber, the slit width of the monochroma
(Number wheels below each of these parameters allow you to change the
analytical curves change dynamically as the variables are changed). The c
different least-squares methods, shown from left to right:

1. A first-order (straight line) fit of measured absorbance (y-axis) vs co
common and straightforward method, but it obviously can not compensa
performed using the SLOPE and INTERCEPT functions (on Sheet2 in c
concentration of unknown samples is given by (A - intercept) / slope wh
slope and intercept from the first-order fit.

ares curve fitting to absorption
ty due to polychromaticity and
ion is similar to "Instrumental Deviation
nalytical curve (absorbance vs
ns measured in an absorption
y light, given the maximum absorptivity,
ator, and the percent stray light.
e values quickly without typing. The
calibration curve is fit using three

oncentration (x-axis). The is the most
ate for non-linearity. This fit is
cells G51, G52, and G53). The
ere A is the measured absorbance and