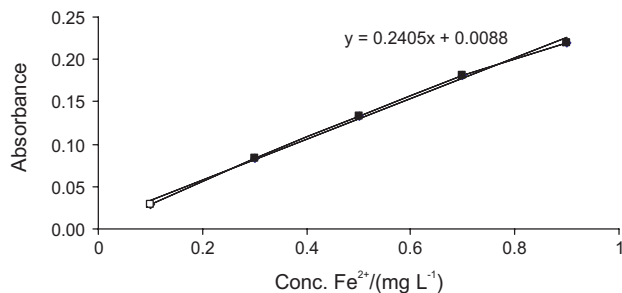*Supplementary Information*

Uncertainties Related to Linear Calibration Curves: A Case Study for Flame Atomic Absorption Spectrometry

Queenie S. H. Chui[*]

*Programa de Pós-Graduação em Engenharia e Ciência dos Materiais, Universidade São Francisco,
Rua Alexandre Rodrigues Barbosa, 45, 13250-901 Itatiba-SP, Brazil*

Although not regarding the experiment under consideration, an example of a calibration with correlation coefficient close to +1 and linearity test not accepted is showed. The raw data for an analytical curve of iron (from 0.1 to 0.9 mg L^{-1}) are presented in Table S1. The analysis of variance is presented in Table S2. It can be seen that there is lack-of-fit even when $R^2 = 0.9941$ (Table S3) with

$F_{calculated}$ (5.14) > $F_{critical}$ (3.71) at 0.05 significance level test. By eliminating data related to the lowest concentration, the statistical tests are repeated and the linear model adjusted. For the range of 0.3 to 0.9 mg L^{-1}, $R^2 = 0.9914$ and $F_{calculated}$ (2.80) < $F_{critical}$ (4.46) at 0.05 significance level test are observed in Table S3. The graphic and the equation calculated by the EXCEL software is in Figure S1.

$y = 0.2405x + 0.0088$

Figure S1. Curve Absorbance *versus* Concentration – an example of a lack-of-fit calibration.

Table S1. Raw data for iron determination – an example to illustrate a lack-of-fit calibration with R^2 close to +1

Conc. Fe^{2+}/(mg L^{-1})	Absorbance units		
0.1	0.28	0.29	0.29
0.3	0.84	0.83	0.81
0.5	0.135	0.131	0.135
0.7	0.180	0.181	0.183
0.9	0.215	0.230	0.216

Table S2. Analysis of variance for 0.1 to 0.9 mg L^{-1} and 0.3 to 0.9 mg L^{-1} ranges of Conc. Fe^{2+}

(iron analytical curve: 0.1 to 0.9 mg L^{-1})				
Sources of Variability	Sum of Squares(SQ)	Degrees of Freedom	Mean Sum of Squares(MQ)	
Totals	0.321014	15	0.021401	MQT
Corrected	0.070107	14	0.005008	MQC
Regression	0.069697	1	0.069697	MQR
Residual	0.000410	13	3.154E-05	MQE
Pure Error	0.000161	10	1.613E-05	MQEP
Lack-of-Fit	0.000249	3	8.293E-05	MQL
(iron analytical curve: 0.3 to 0.9 mg L^{-1})				
Totals	0.318548	12	0.026546	MQT
Corrected	0.032105	11	0.002919	MQC
Regression	0.031832	1	0.031832	MQR
Residual	0.000273	10	2.729E-05	MQE
Pure Error	0.000161	8	2.008E-05	MQEP
Lack-of-Fit	0.000112	2	5.613E-05	MQL

*e-mail: queenie.hang@saofrancisco.edu.br

Table S3. Results of linearity and regression efficiency tests (for 0.1 to 0.9 mg L^{-1} and 0.3 to 0.9 mg L^{-1} ranges of Conc. Fe^{2+})

(iron analytical curve: 0.1 to 0.9 mg L^{-1})	
Linearity (lack-of-fit)	Is "a" $\neq$ zero?
$F_{calculated} = MQL / MQEP = 5.14$	$F_{calculated} = MQR / MQE = 2209$
$F_{3; 10; 0.05} = 3.71$	$F_{1; 13; 0.05} = 4.67$
$F_{calculated} > F_{3; 10; 0.05}$	$F_{calculated} \gg F_{1; 13; 0.05}$
Linearity is not accepted	"a" $\neq$ zero
Efficiency	Maximum Efficiency
$R^2 = SQR / SQC = 0.9941$	$R^2_{max} = (SQC - SQEP) / SQC$
	$R^2_{max} = 0.9977$

(iron analytical curve: 0.3 to 0.9 mg L^{-1})	
Linearity (lack-of-fit)	Is "a" $\neq$ zero?
$F_{calculated} = MQL / MQEP = 2.80$	$F_{calculated} = MQR / MQE = 1166$
$F_{2; 8; 0.05} = 4.46$	$F_{1; 13; 0.05} = 4.96$
$F_{calculated} < F_{2; 8; 0.05}$	$F_{calculated} \gg F_{1; 10; 0.05}$
Linearity is accepted	"a" $\neq$ zero
Efficiency	Maximum Efficiency
$R^2 = SQR / SQC = 0.9914$	$R^2_{max} = (SQC - SQEP) / SQC$
	$R^2_{max} = 0.9950$