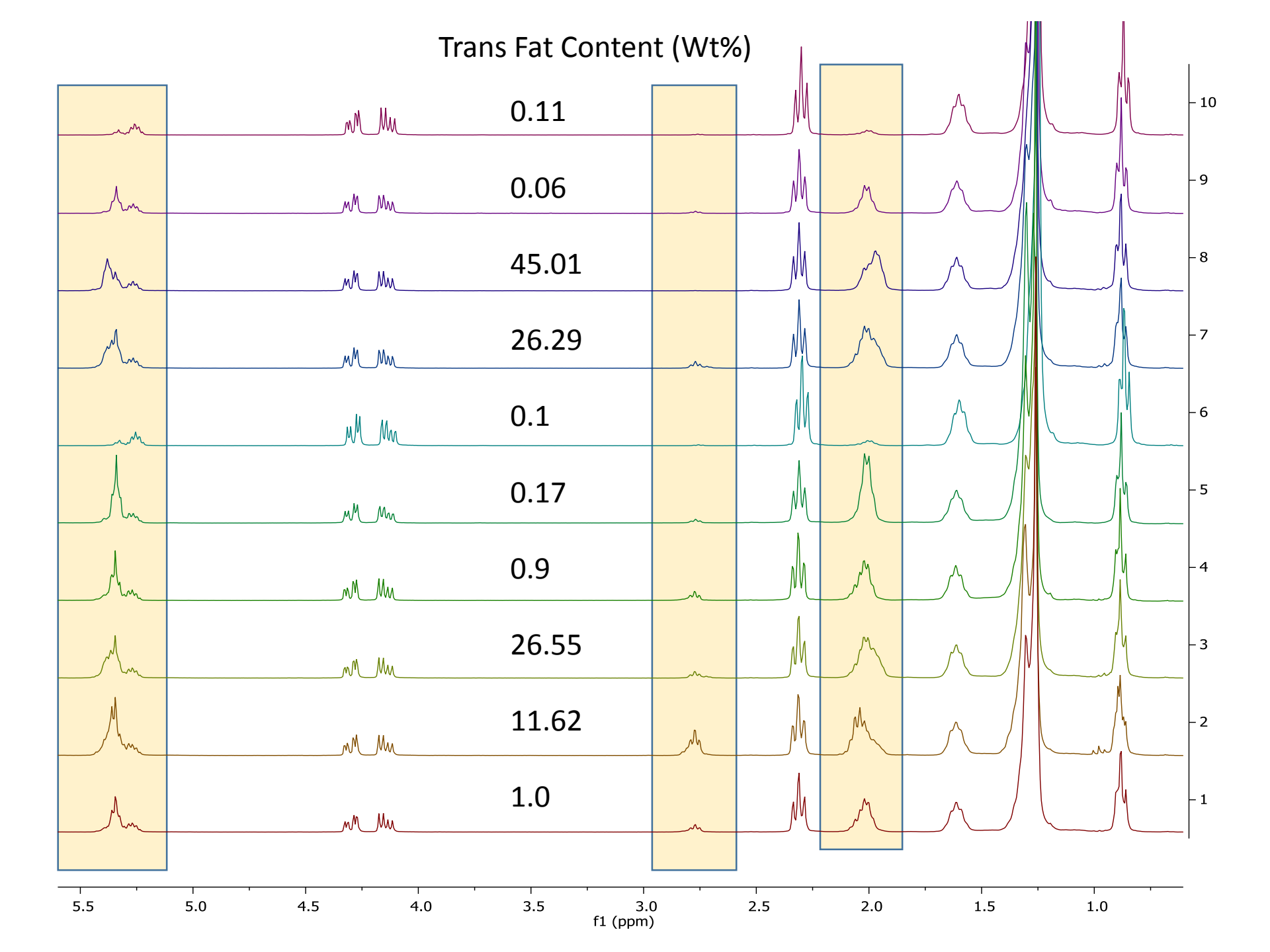

Trans Fat Content (Wt%)
0.11
0.06
45.01
26.29
0.1
0.17
0.9
26.55
11.62
1.0
10
9
8
7
6
5
4
3
2
1
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

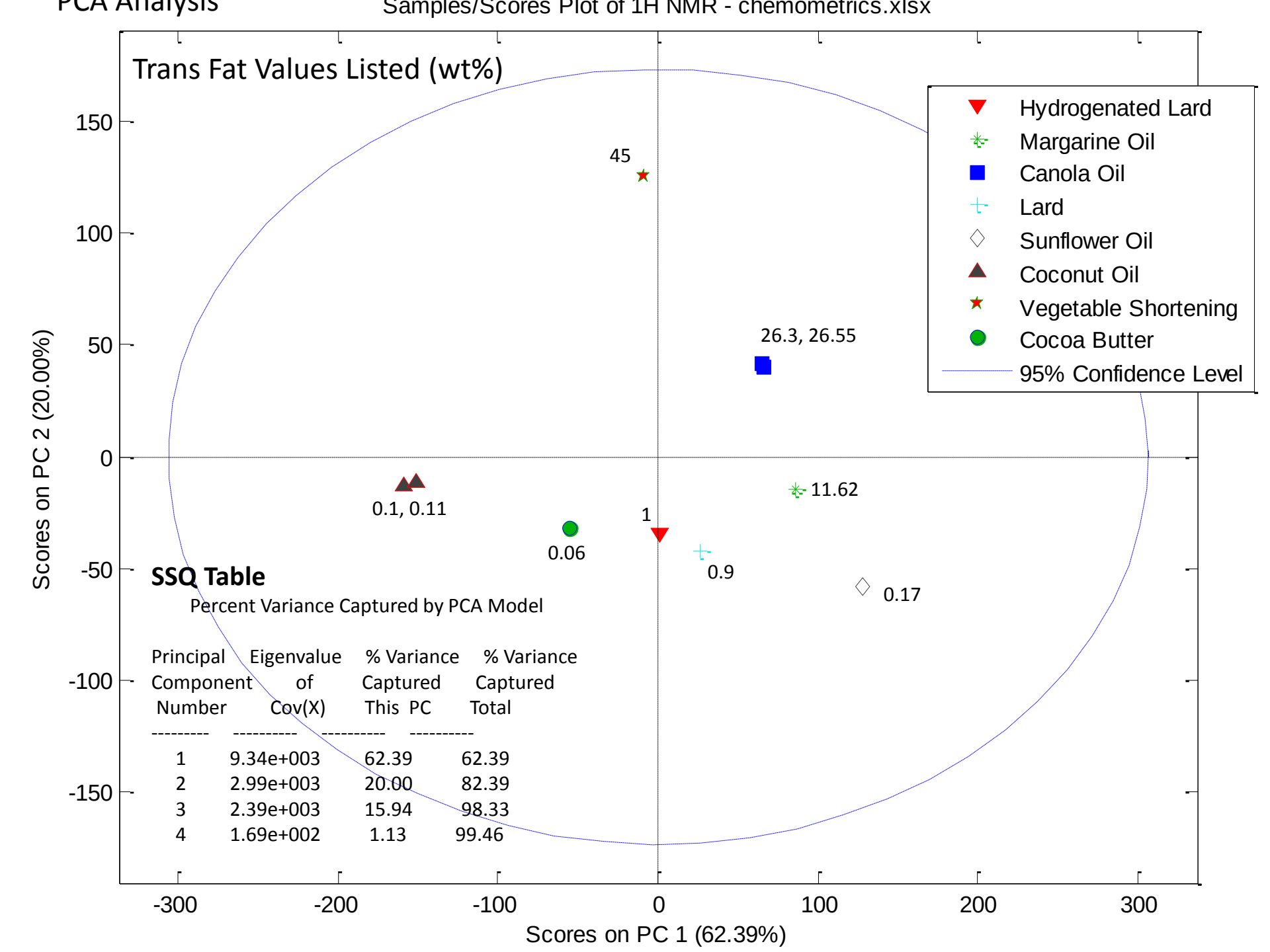
AOCS – Trans Fat Reference Materials

Sample	Trans Fat	SAFA	MONO	PUFA	Total Fat
Hydrogenated Lard	1	40.27	38.75	12.85	97.39
Margarine Oil	11.62	17.75	21.29	41.7	96.74
Canola Oil	26.55	16.28	39.43	10.7	97.2
Lard	0.9	37.45	40.44	13.29	97.11
Sunflower Oil	0.17	7.51	81	5.41	98.61
Coconut Oil	0.1	84.19	5.32	1.3	96.46
Canola Oil	26.27	16.06	39.23	10.7	96.2
Vegetable Shortening	45.01	23.3	22.57	0.49	95.46
Cocoa Butter	0.06	58.71	32.28	3.12	98.61
Coconut Oil	0.11	84.42	5.25	1.29	96.73

Purchased in Early 2006

1H 300MHz data obtained April 2006
High School Intern Project

NMR Data is binned (0.005ppm) and normalized (area to 10k)


PCA Analysis
Samples/Scores Plot of 1H NMR - chemometrics.xlsx
Trans Fat Values Listed (wt%)
Hydrogenated Lard
Margarine Oil
Canola Oil
Lard
Sunflower Oil
Coconut Oil
Vegetable Shortening
Cocoa Butter
95% Confidence Level
45
26.3, 26.55
0.1, 0.11
11.62
1
0.06
0.9
0.17
SSQ Table
Percent Variance Captured by PCA Model
Principal Component Number
Eigenvalue of Cov(X)
% Variance Captured This PC
% Variance Captured Total
1 9.34e+003 62.39 62.39
2 2.99e+003 20.00 82.39
3 2.39e+003 15.94 98.33
4 1.69e+002 1.13 99.46
150
100
50
0
-50
-100
-150
-300
-200
-100
0
100
200
300
Scores on PC 2 (20.00%)
Scores on PC 1 (62.39%)

Generated by John@JOHN-NEW-HP on 18-Nov-2013 20:16:56

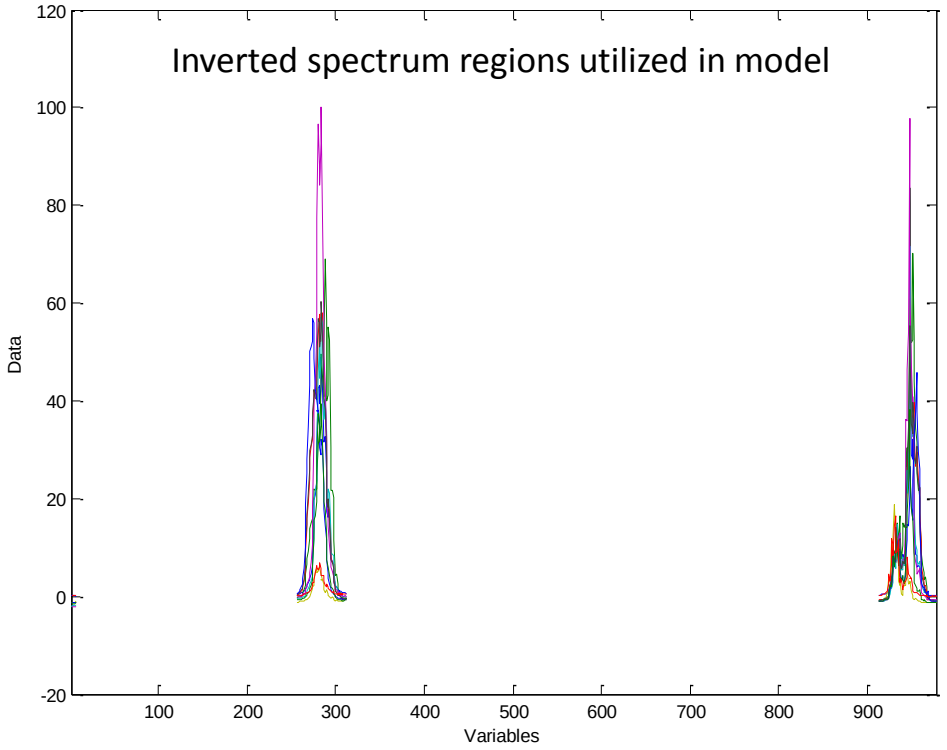
Model

Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 18-Nov-2013 20:13:03.054
Author: John@JOHN-NEW-HP
X-block: 1H NMR - chemometrics.xlsx 10 by 128 (John@JOHN-NEW-HP@2013
m:20131118201231.820)
Included: [1-10] [1-6 256-312 914-978]
Preprocessing: Mean Center
Y-block: trans fat values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131118T2010
m:20131118201231.830)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 3
Cross validation: venetian blinds w/ 3 splits
RMSEC: 0.570994
RMSECV: 1.19476
Bias: 1.77636e-015
CV Bias: 0.162888
R^2 Cal: 0.998587
R^2 CV: 0.994364

SSQ Table

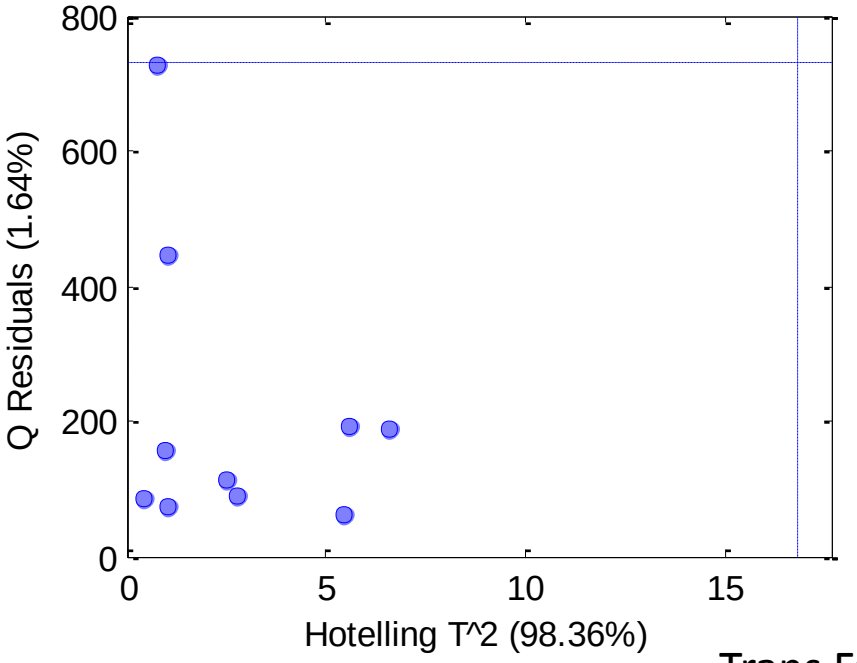
Percent Variance Captured by Regression Model

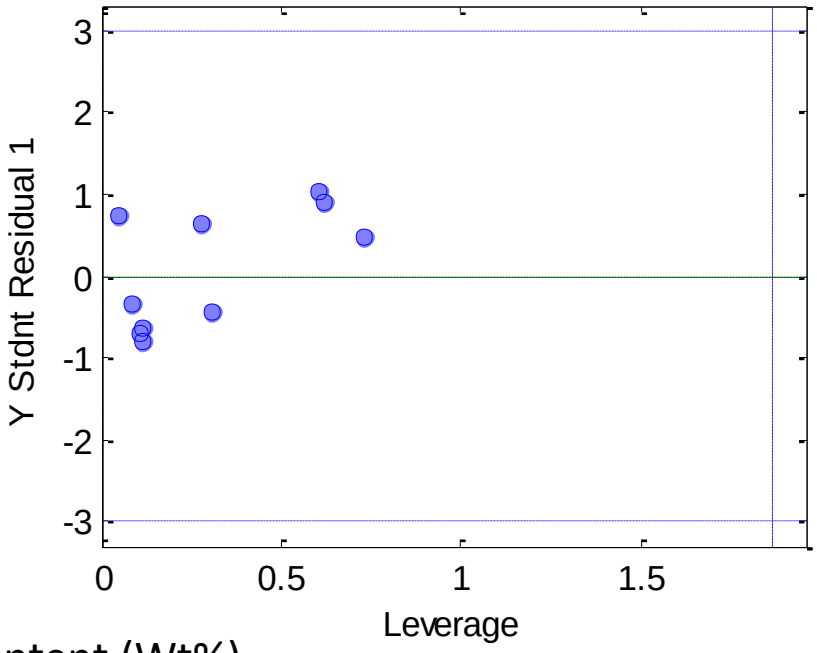
	-----X-Block-----		-----Y-Block-----	
Comp	This	Total	This	Total
1	41.85	41.85	79.40	79.40
2	42.76	84.61	20.41	99.81
3	13.75	98.36	0.05	99.86



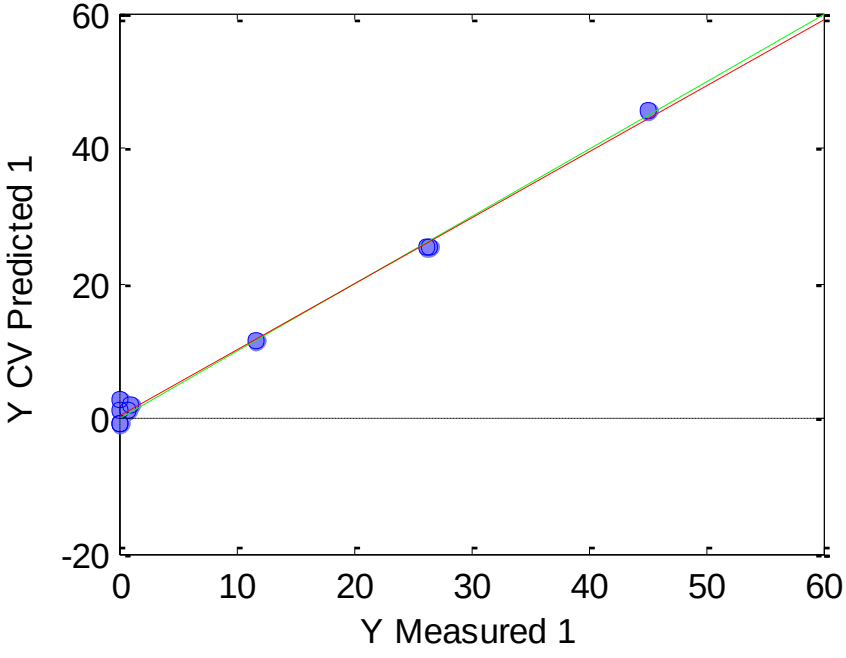
Trans Fat Analysis by 1H NMR (300 MHz) – PLS Regression

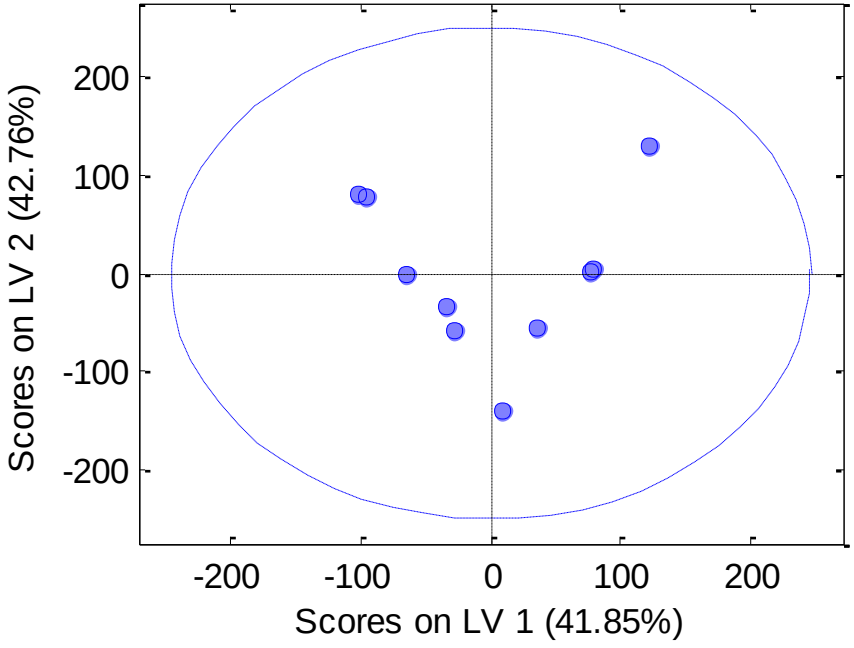
2 Region Correlation – 3 Factors - R2=0.994 SECV = 1.19 wt%
Model Range 0-45%





Trans Fat Content (Wt%)



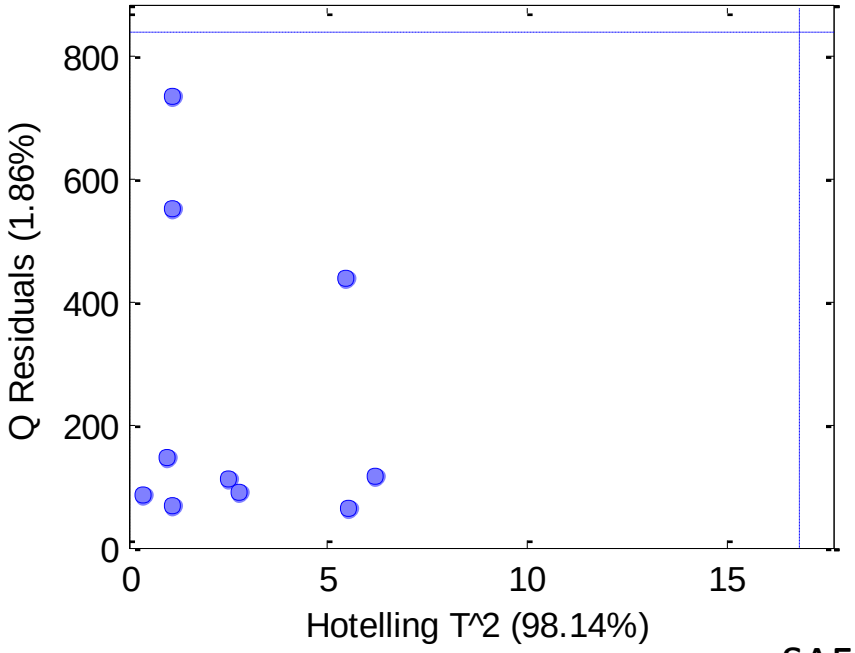


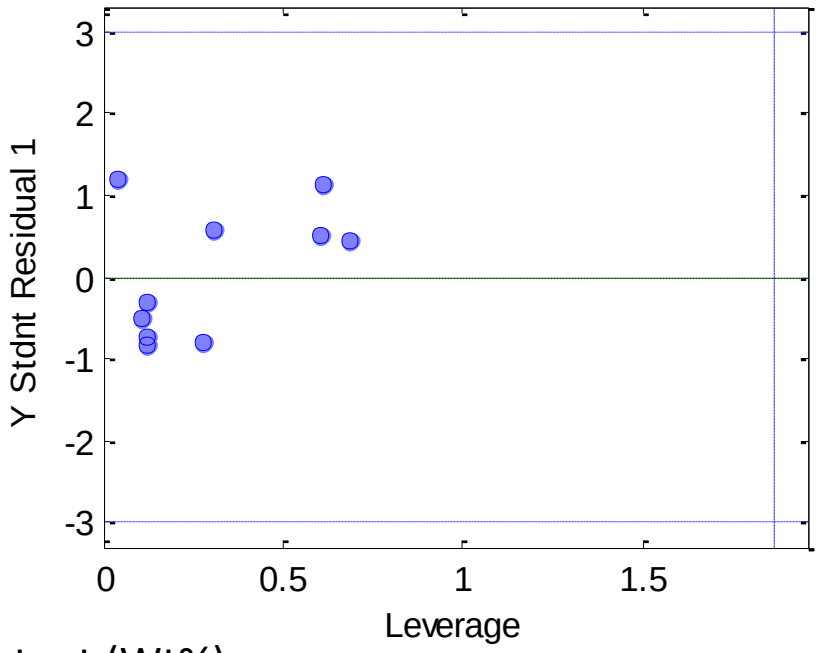
SAFA Analysis

Generated by John@JOHN-NEW-HP on 18-Nov-2013 20:53:14

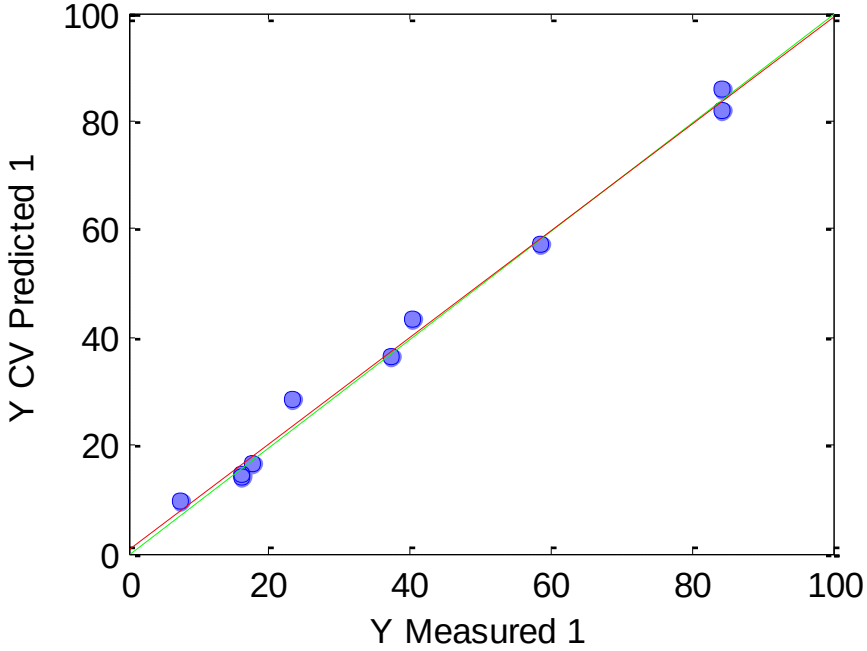
Model

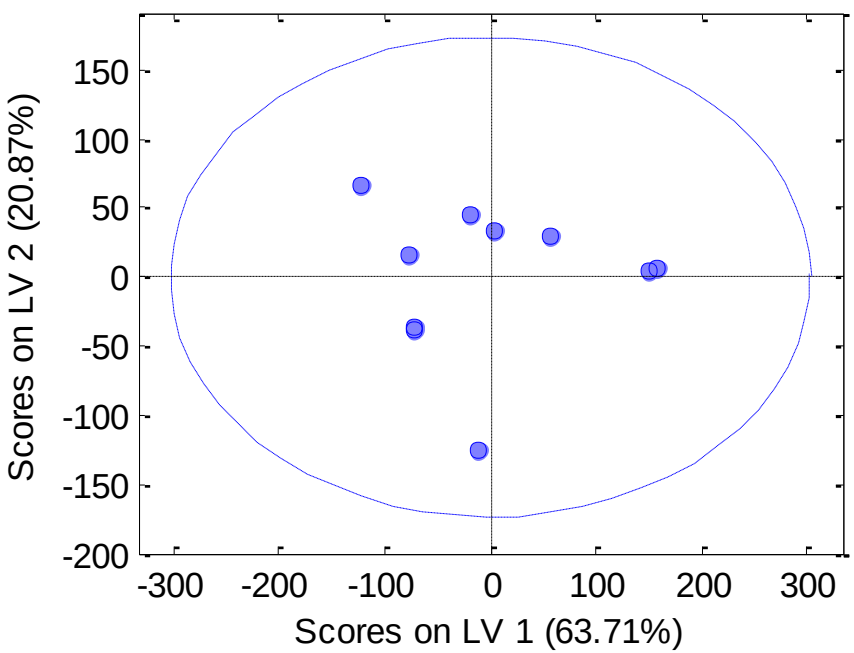
Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 18-Nov-2013 20:51:039.74
Author: John@JOHN-NEW-HP
X-block: 1H NMR - chemometrics.xlsx 10 by 128 (John@JOHN-NEW-HP@20131118T201007.82955246 m:20131118201231.820)
Included: [1-10] [1-6 256-312 914-978]
Preprocessing: Mean Center
Y-block: SAFA values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131118T205125.66667115 m:20131118205125.676)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 3
Cross validation: leave one out
RMSEC: 1.3137
RMSECV: 2.48908
Bias: 0
CV Bias: 0.229265
R^2 Cal: 0.997612
R^2 CV: 0.991566





SAFA Content (Wt%)



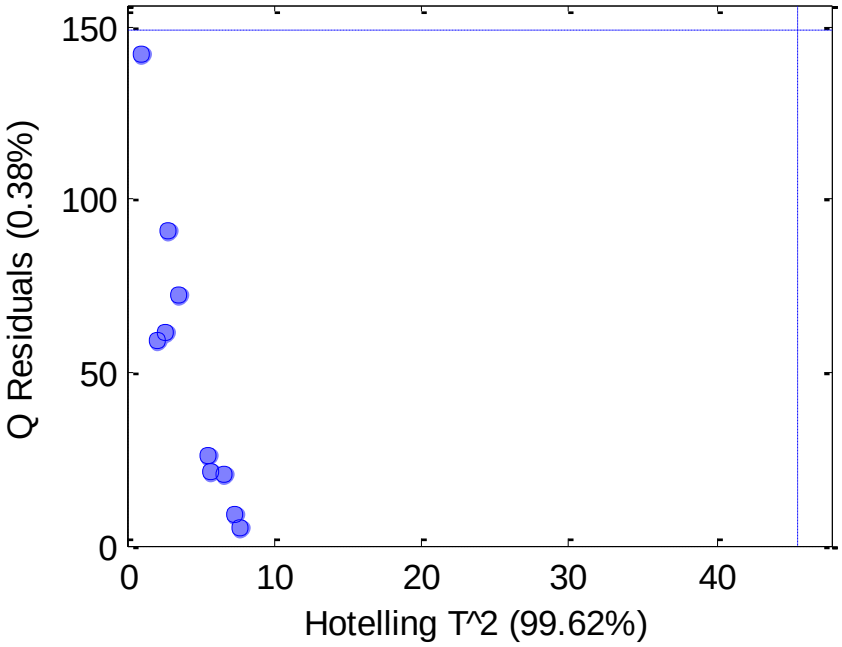


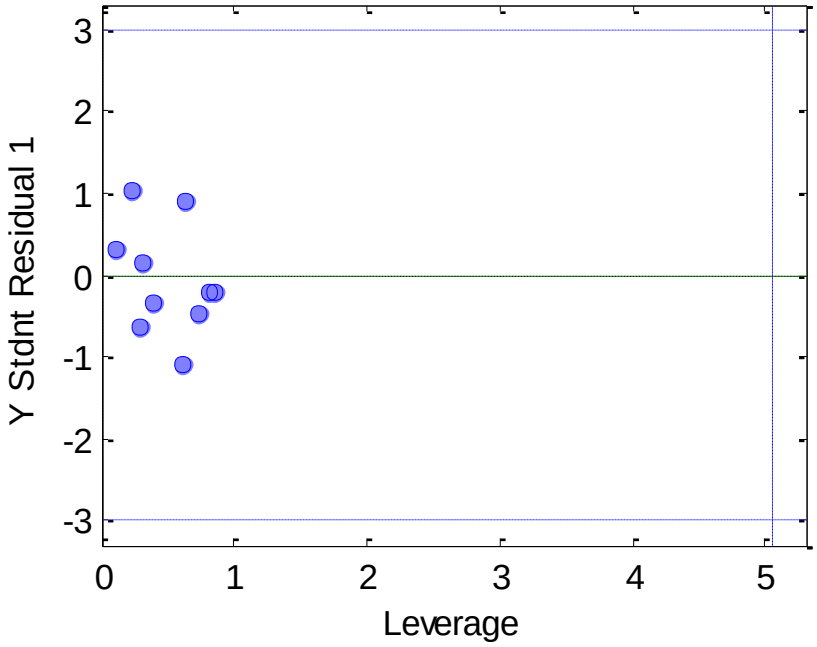
Mono Unsaturated Content (wt%)

Generated by John@JOHN-NEW-HP on 18-Nov-2013 21:06:15

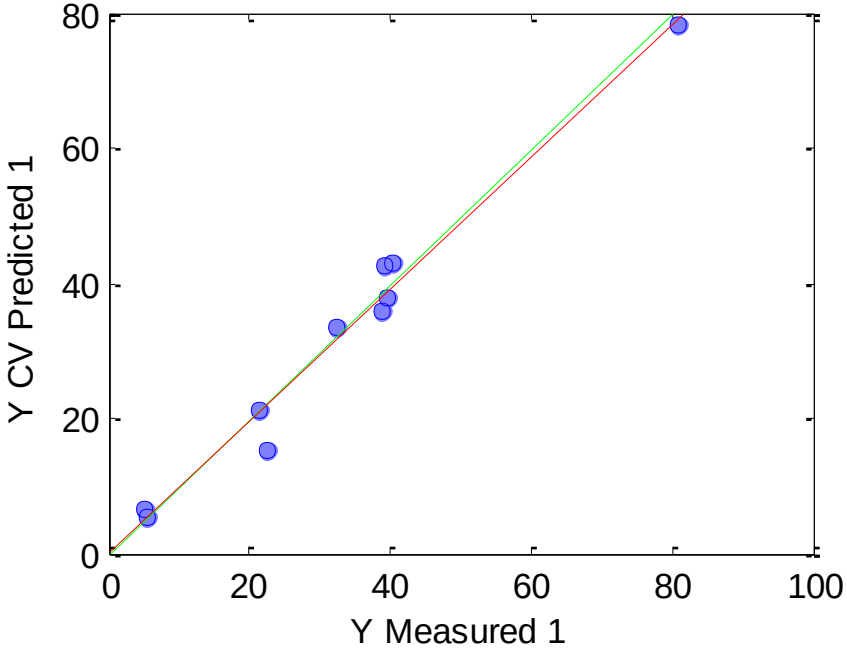
Model

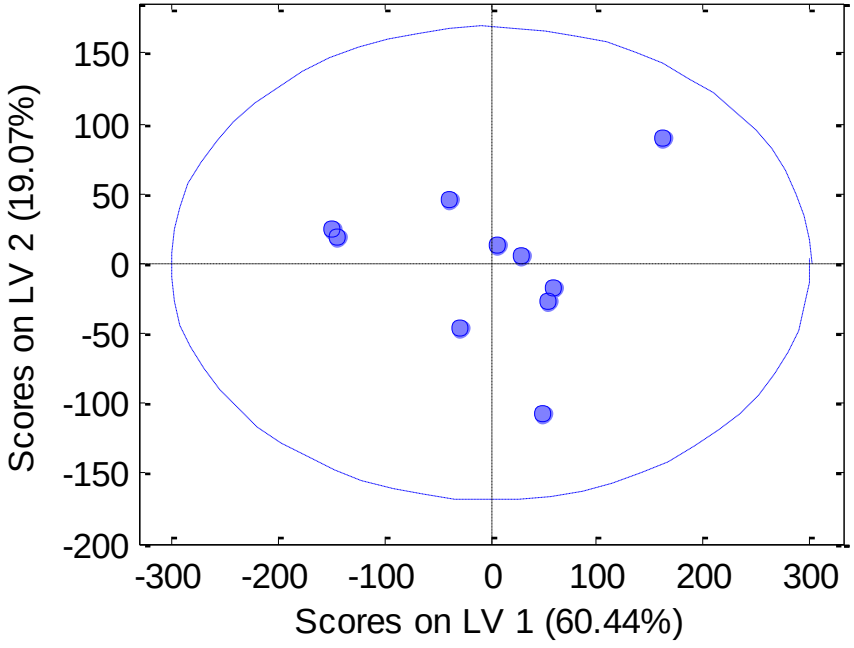
Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 18-Nov-2013 21:05:029.36
Author: John@JOHN-NEW-HP
X-block: 1H NMR - chemometrics.xlsx 10 by 165 (John@JOHN-NEW-HP@20131118T210141.42857313 m:20131118210505.321)
Included: [1-10] [254-313 422-459 909-975]
Preprocessing: Mean Center
Y-block: MONO values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131118T210302.63809165 m:20131118210505.331)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 5
Cross validation: leave one out
RMSEC: 0.742692
RMSECV: 3.05967
Bias: 0
CV Bias: -0.621651
R^2 Cal: 0.998703
R^2 CV: 0.978898





MonoUnsaturated Content (Wt%)



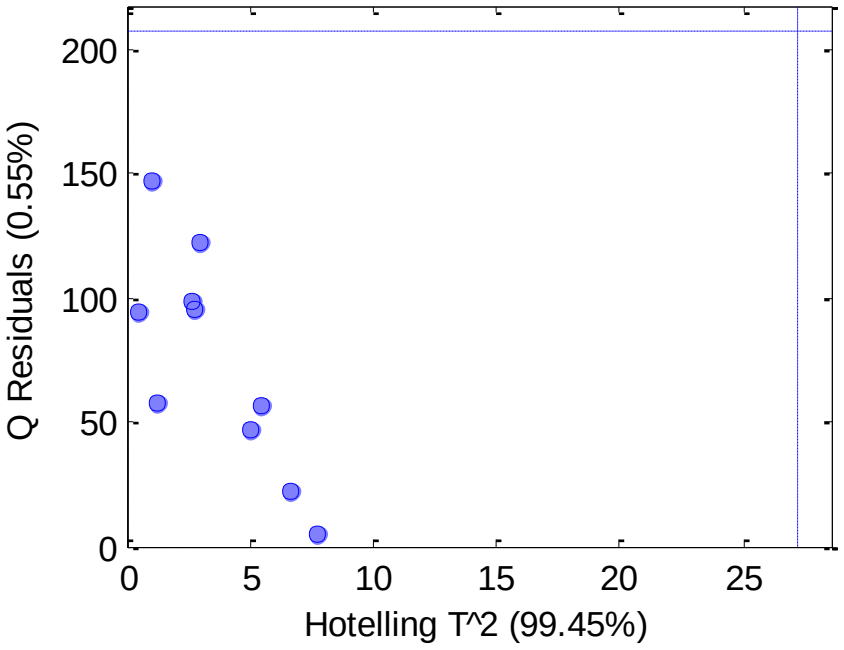


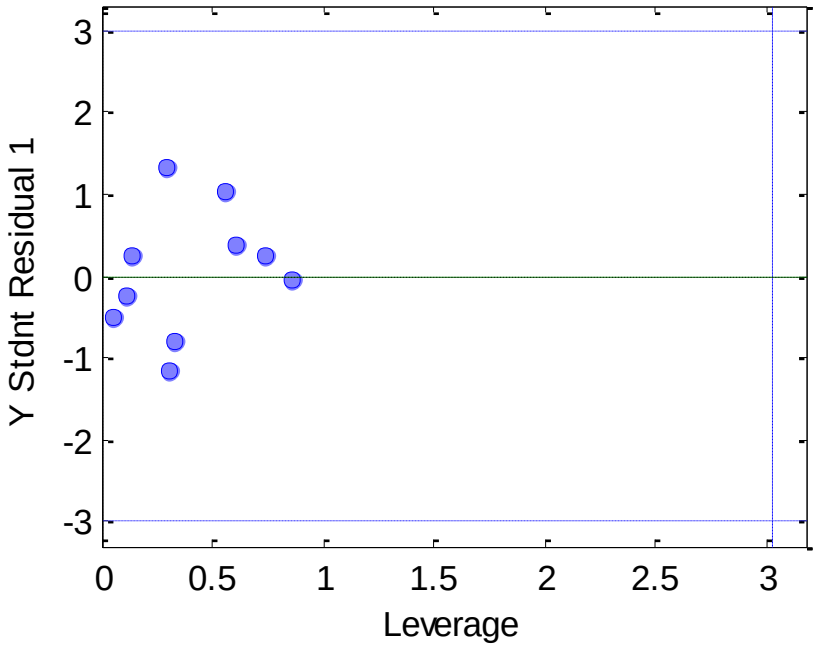
PUFA Analysis

Generated by John@JOHN-NEW-HP on 18-Nov-2013 21:09:51

Model

Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 18-Nov-2013 21:08:046.12
Author: John@JOHN-NEW-HP
X-block: 1H NMR - chemometrics.xlsx 10 by 165 (John@JOHN-NEW-HP@20131118T210141.42857313 m:20131118210505.321)
Included: [1-10] [254-313 422-459 909-975]
Preprocessing: Mean Center
Y-block: PUFA values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131118T210832.34656487 m:20131118210832.366)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 4
Cross validation: leave one out
RMSEC: 0.450612
RMSECV: 1.72043
Bias: 1.77636e-015
CV Bias: -0.210782
R^2 Cal: 0.998479
R^2 CV: 0.987062





PUFA Content (Wt%)