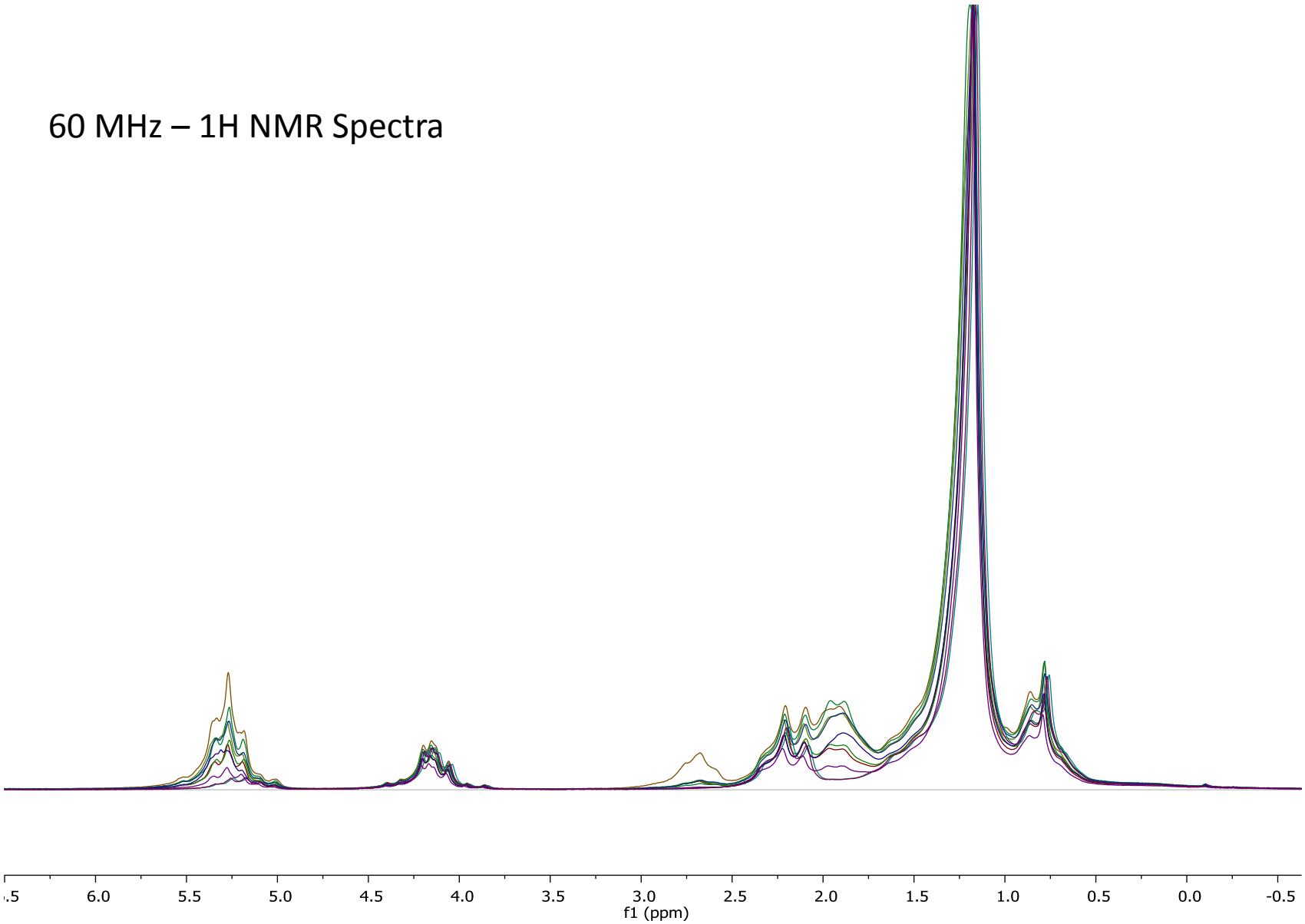
60 MHz – 1H NMR Spectra



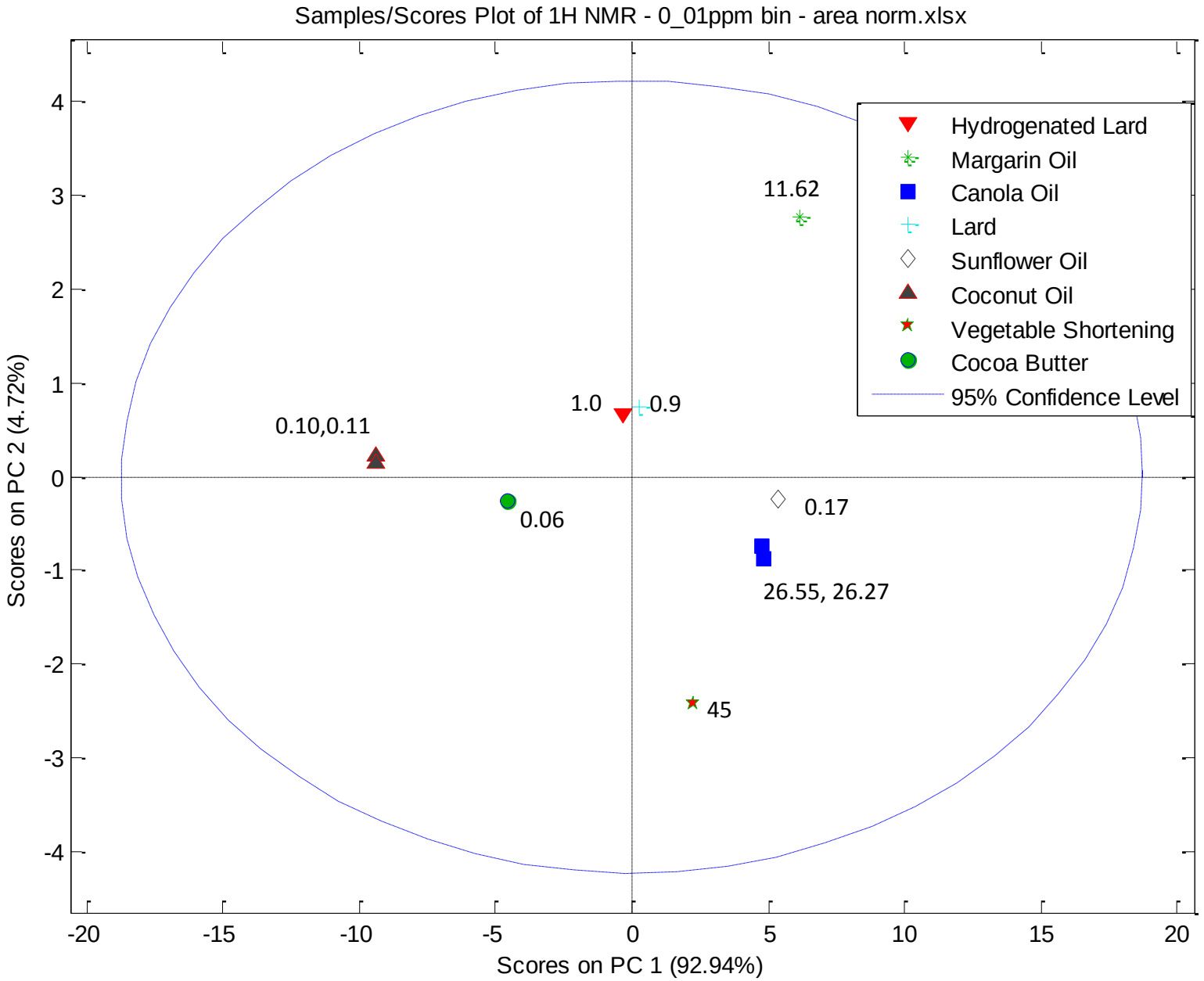
AOCS – Trans Fat Reference Materials

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 60 MHz data obtained April 2006
High School Intern Project

PCA Analysis – Full Spectrum



Analysis Report Trans Fat Content (Wt%)

Generated by John@JOHN-NEW-HP on 20-Nov-2013 11:42:54

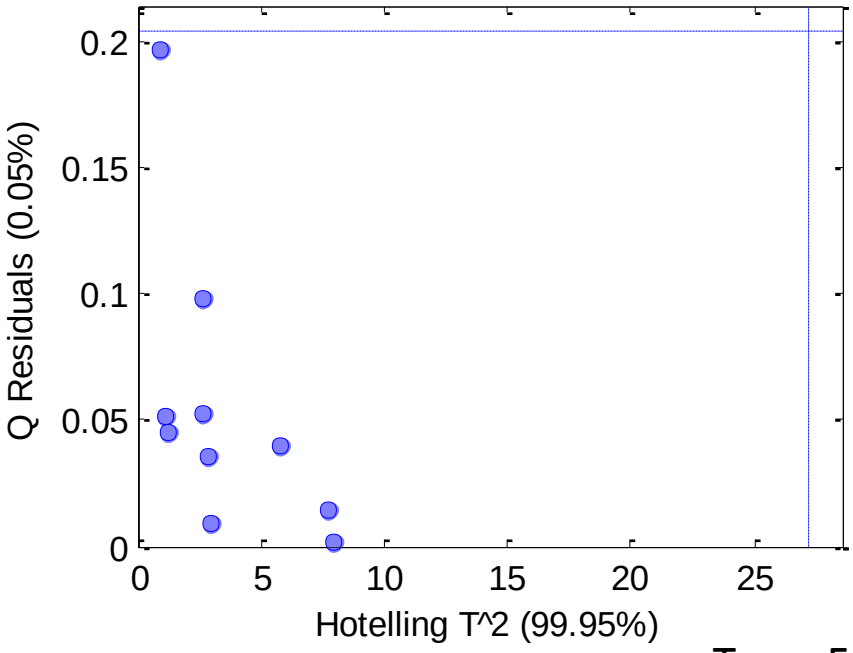
Model

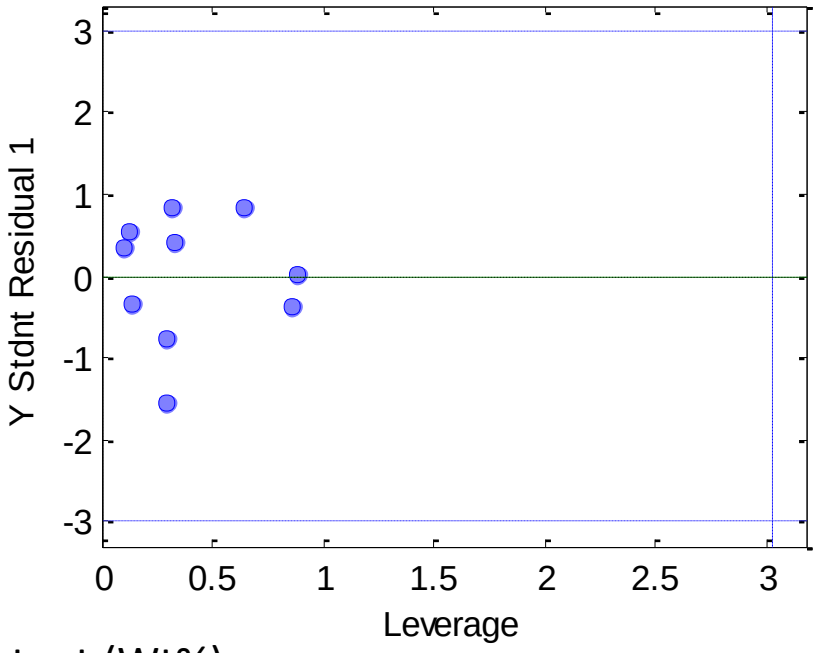
Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 20-Nov-2013 10:50:057.54
Author: John@JOHN-NEW-HP
X-block: Multiple SPC Files 10 by 35 (John@JOHN-NEW-HP@20131120T104547.81302599 m:20131120104905.766)
Included: [1-10] [10-34 117-126]
Included (in axis units): [n/a] [10-34 117-126]
Preprocessing: Mean Center
Y-block: trans fat values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131120T104618.88999481 m:20131120104905.782)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 4
Cross validation: leave one out
RMSEC: 0.208695
RMSECV: 1.46124
Bias: -1.77636e-015
CV Bias: -0.256664
R^2 Cal: 0.999811
R^2 CV: 0.991072

SSQ Table

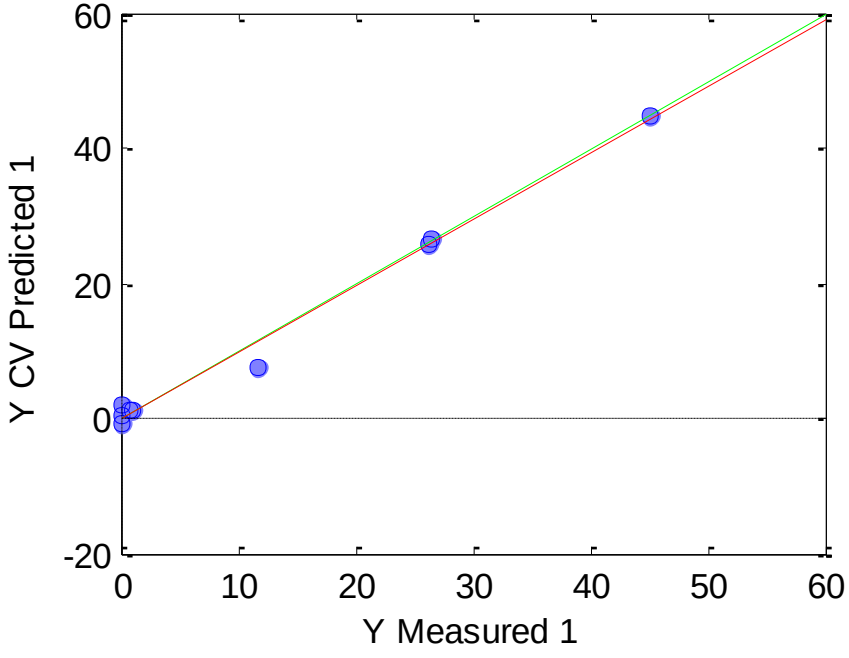
Percent Variance Captured by Regression Model

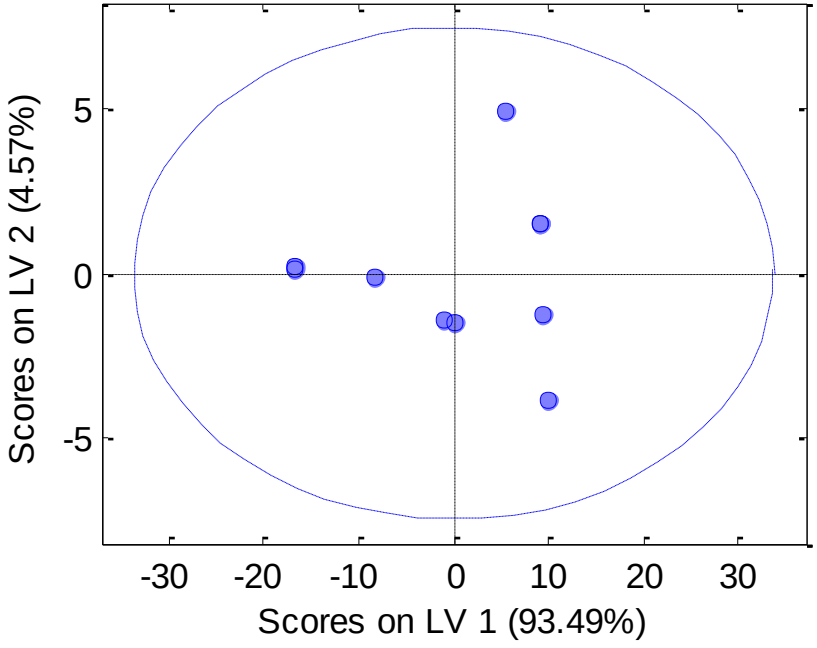
	-----X-Block-----		-----Y-Block-----	
Comp	This	Total	This	Total
1	93.49	93.49	29.86	29.86
2	4.57	98.06	55.26	85.12
3	1.72	99.78	14.68	99.79
4	0.17	99.95	0.19	99.98





Trans Fat Content (Wt%)





Analysis Report PUFA Content (Wt%)

Generated by John@JOHN-NEW-HP on 20-Nov-2013 11:57:00

Model

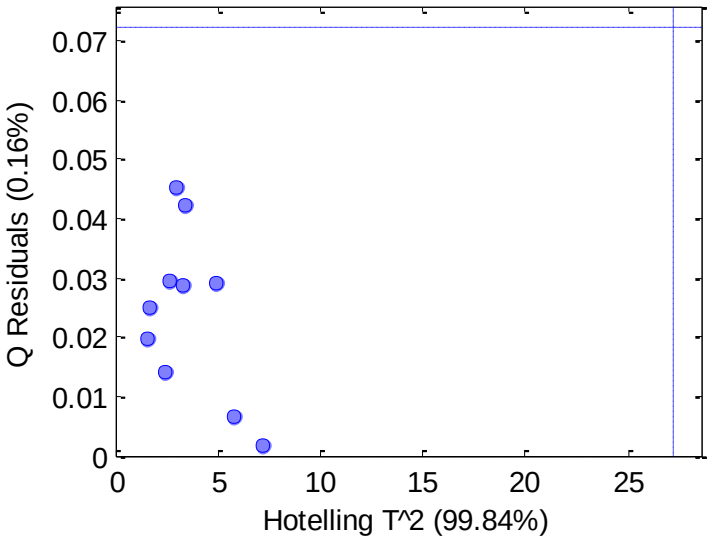
Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 20-Nov-2013 11:56:000040
Author: John@JOHN-NEW-HP
X-block: 1H NMR - 0_01ppm bin - area norm.xlsx 10 by 220 (John@JOHN-NEW-HP@20131120T115421.49480915 m:20131120115616.108)
Included: [1-10] [201-304 435-550]
Preprocessing: Mean Center
Y-block: PUFA values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131120T115434.61450789 m:20131120115616.124)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 4
Cross validation: leave one out
RMSEC: 0.243444
RMSECV: 0.563559
Bias: 0
CV Bias: 0.095792
R^2 Cal: 0.999556
R^2 CV: 0.997755

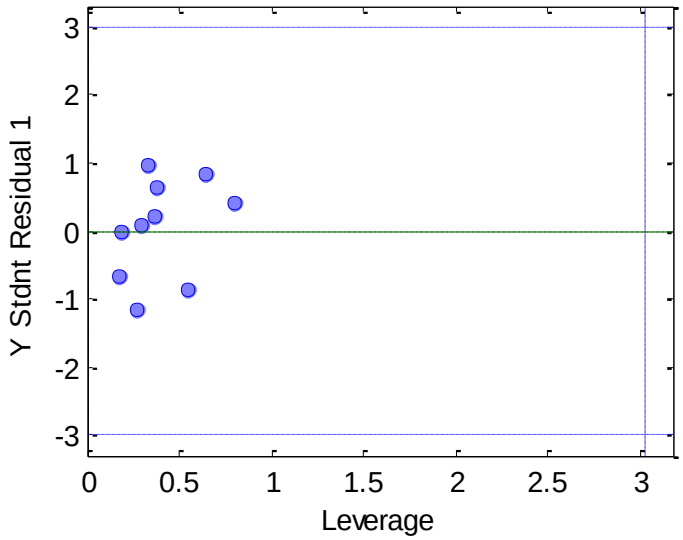
SSQ Table

Percent Variance Captured by Regression Model

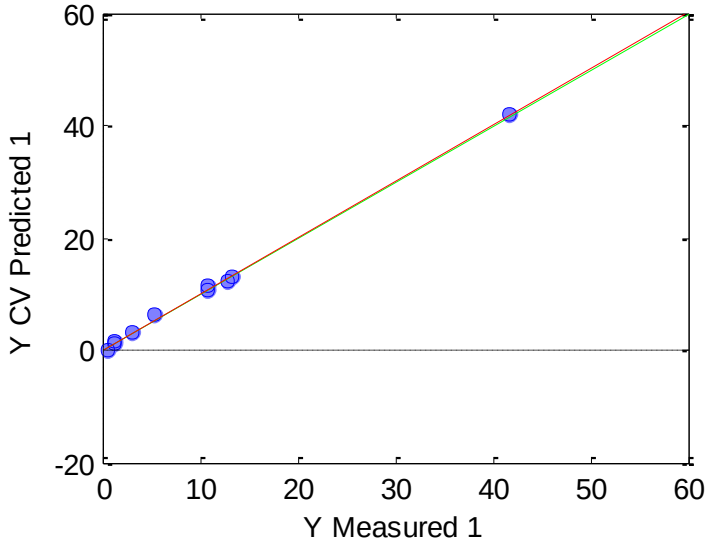
	-----X-Block-----		-----Y-Block-----	
Comp	This	Total	This	Total
1	89.01	89.01	65.13	65.13
2	7.14	96.15	32.92	98.05
3	3.06	99.21	1.86	99.90
4	0.63	99.84	0.05	99.96

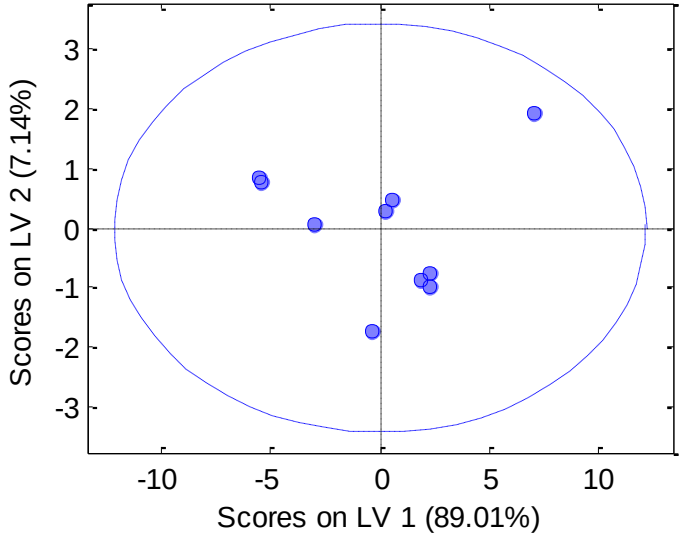
There is 1 figure associated with this analysis





PUFA Content (Wt%)





Analysis Report SAFA Content (Wt%)

Generated by John@JOHN-NEW-HP on 20-Nov-2013 12:00:27

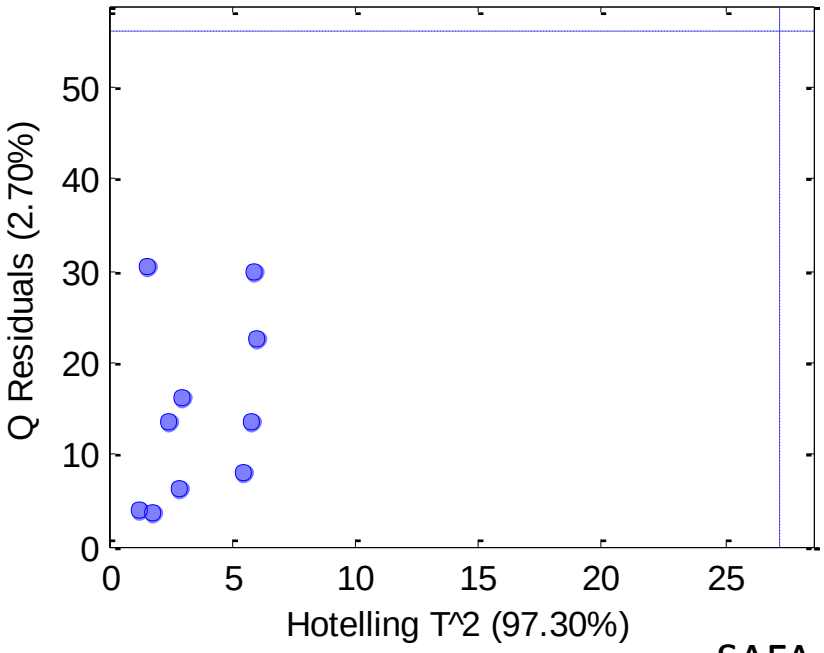
Model

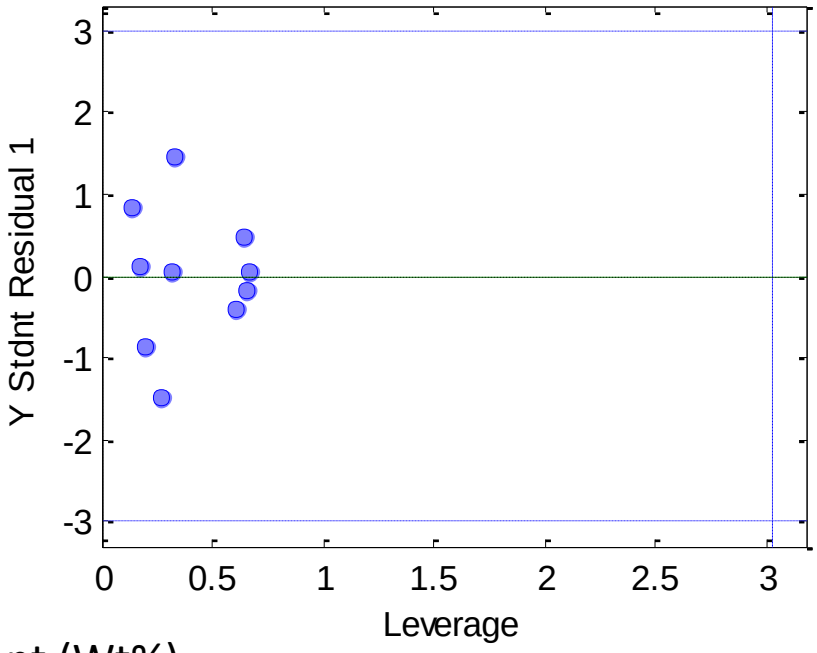
Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 20-Nov-2013 11:59:059.31
Author: John@JOHN-NEW-HP
X-block: 1H NMR - 0_01ppm bin - area norm.xlsx 10 by 550 (John@JOHN-NEW-HP@20131120T114626.33978362 m:20131120114626.339)
Included: [1-10] [1-550]
Preprocessing: Mean Center
Y-block: SAFA values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131120T114638.28985324 m:20131120114638.304)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 4
Cross validation: leave one out
RMSEC: 0.695404
RMSECV: 6.36181
Bias: 0
CV Bias: -0.377895
R^2 Cal: 0.999331
R^2 CV: 0.945848

SSQ Table

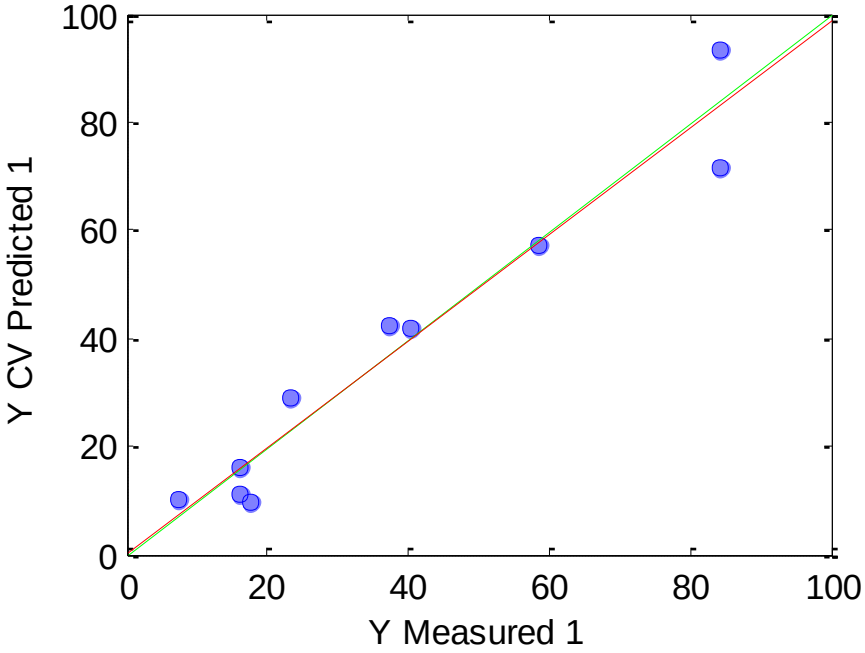
Percent Variance Captured by Regression Model

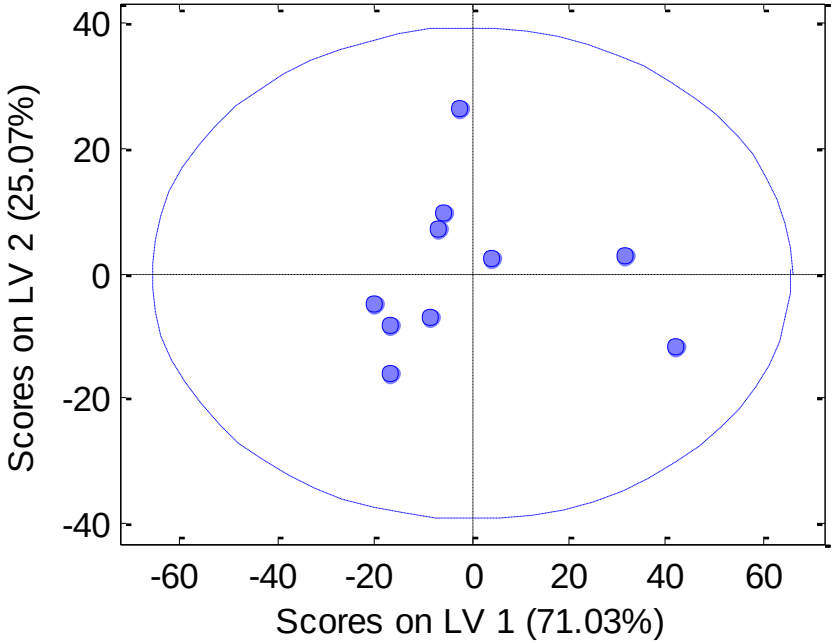
	-----X-Block-----		-----Y-Block-----	
Comp	This	Total	This	Total
1	71.03	71.03	85.46	85.46
2	25.07	96.11	7.83	93.29
3	0.73	96.84	6.27	99.56
4	0.46	97.30	0.37	99.93





SAFA Content (Wt%)





Analysis Report MONO Content (Wt%)

Generated by John@JOHN-NEW-HP on 20-Nov-2013 12:07:53

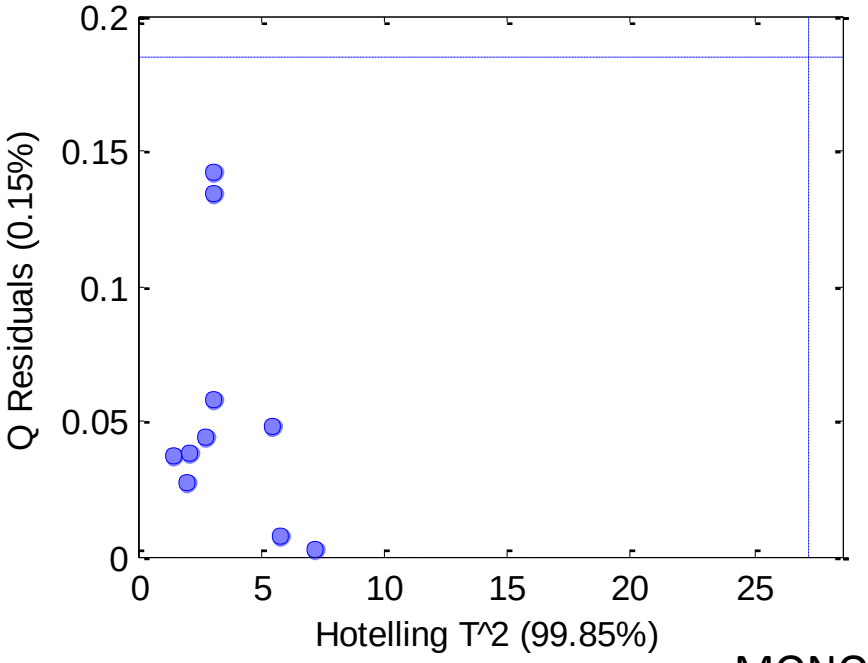
Model

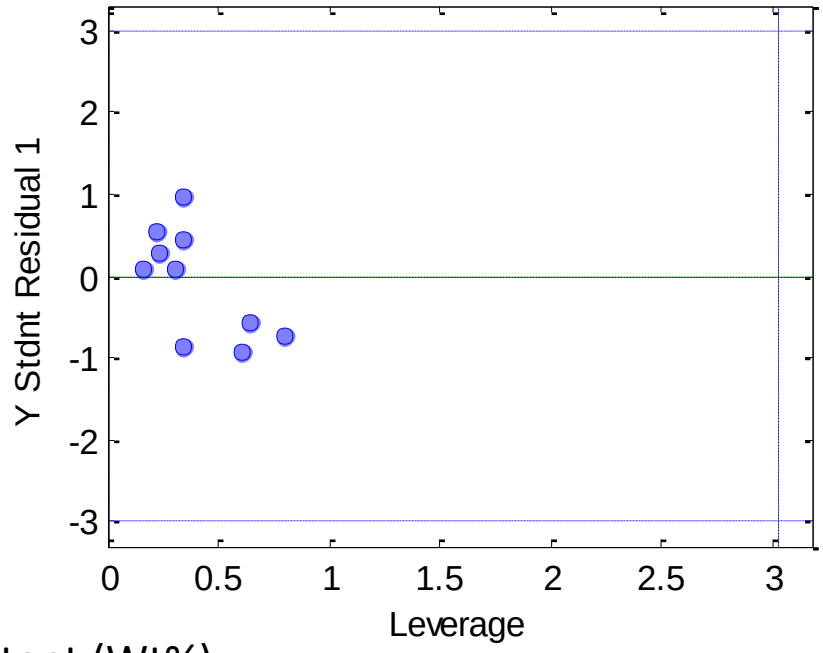
Linear regression model using
Partial Least Squares calculated with the SIMPLS algorithm
Developed 20-Nov-2013 12:06:000028
Author: John@JOHN-NEW-HP
X-block: 1H NMR - 0_01ppm bin - area norm.xlsx 10 by 221 (John@JOHN-NEW-HP@20131120T120336.63916248 m:20131120120605.334)
Included: [1-10] [124-154 206-279 435-550]
Preprocessing: Mean Center
Y-block: MONO values.xlsx 10 by 1 (John@JOHN-NEW-HP@20131120T120349.29134379 m:20131120120605.350)
Included: [1-10] [1]
Preprocessing: Mean Center
Num. LVs: 4
Cross validation: leave one out
RMSEC: 1.72044
RMSECV: 5.45103
Bias: -7.10543e-015
CV Bias: -1.60478
R^2 Cal: 0.993041
R^2 CV: 0.936347

SSQ Table

Percent Variance Captured by Regression Model

	-----X-Block-----		-----Y-Block-----	
Comp	This	Total	This	Total
1	89.67	89.67	43.44	43.44
2	6.53	96.20	30.85	74.29
3	3.08	99.28	21.91	96.20
4	0.57	99.85	3.10	99.30





MONO Content (Wt%)