

PROCESS NMR ASSOCIATES

Utilization of MNova in a Commercial NMR Testing Laboratory for :

- 1) Development of Automated Quantitative Analysis Methods by Direct Internal Standard NMR Measurements, and**
- 2) Pre-Processing of Large NMR Datasets for Chemometric Regression Analyses to Derive Chemical and Physical Properties**

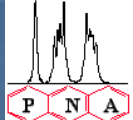
John Edwards

Process NMR Associates, LLC, Danbury, Connecticut

September 22, 2013

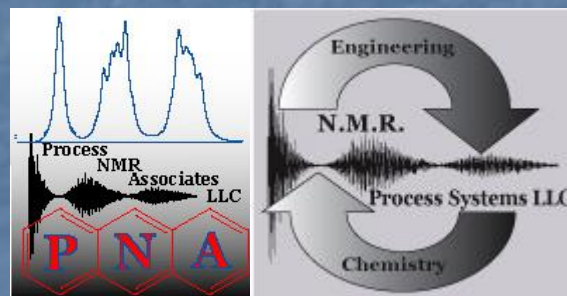
MestreLab MNova Users Meeting, SMASH 2013

Santiago de Compostela, Spain



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250+ Analytical NMR Customers



TTC Labs, Inc.
Process Engineering Excellence

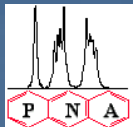


**Analytical
Services
And
Consulting**



TopNIR Systems





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Quantitative ^1H qNMR Method for Complex Mixture Analysis: Determination of Acetylated Polysaccharides, Glucose, Maltodextrin, Isocitrate, Malic Acid in Aloe Vera Leaf Juice.

Also ... Preservatives, Additives, and Degradation Products in Aloe Vera Raw Materials and Consumer Products

Presented By

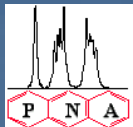
John Edwards, Ph.D.

**Process NMR As
sociates, LLC**

Danbury, Connecticut

November 9, 2012 Aloe Summit, Las Vegas, NV

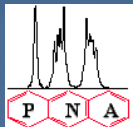
**Development of Automated Quantitative Analysis Methods by Direct Internal
Standard NMR Measurements**



NMR Systems and Experimental Conditions

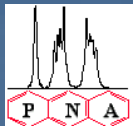
Acquisition Time	3-8 Seconds
Relaxation (Recycle) Delay	2-6 Seconds
Frequency, MHz	300-500 MHz
Nucleus	^1H
Number of Pulse Accumulations*	16-256
Original FID Points	16384-84000
Zero-filled Points	32768-262144
Pulse sequence	Single pulse
Solvent	D_2O
Sweep width, ppm	16
Temperature	Ambient ($25\text{ }^\circ\text{C}$)
Line Broadening	0.35 Hz
Steady State Pulses	8
Pre-Acquisition Delay	60 seconds





Advantages of Using NMR in Complex Mixture Analysis

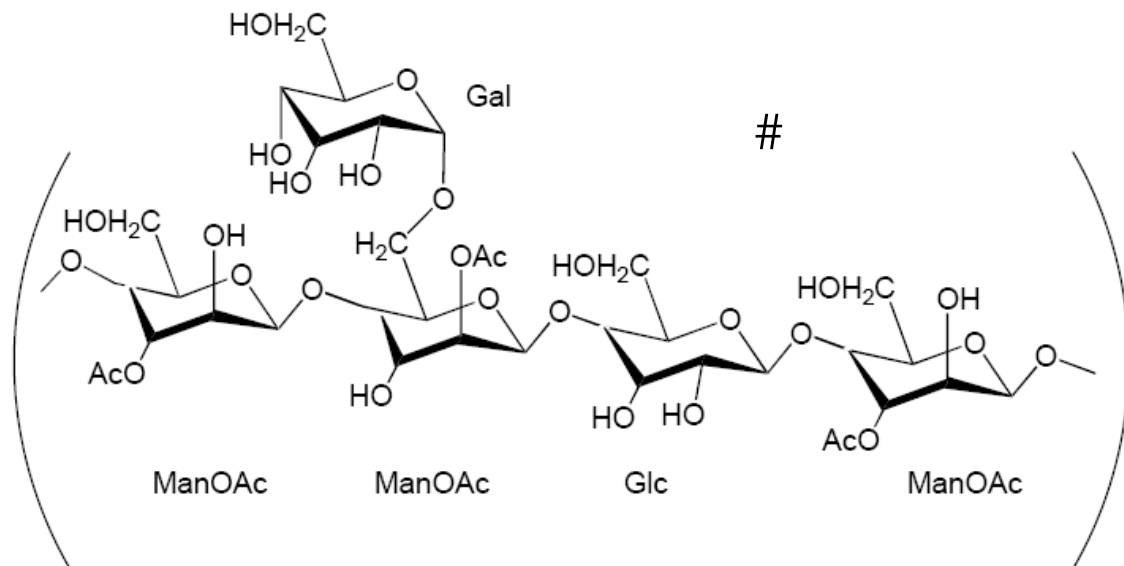
- Minimal Sample Preparation
- Reproducible (site to site, country to country)
- Linear and Quantitative Spectral Response
- Targeted AND Non-Targeted
- Qualitative
- Quantitative
- Compound Specific
- Rapid – 10 Minutes
- Affordable



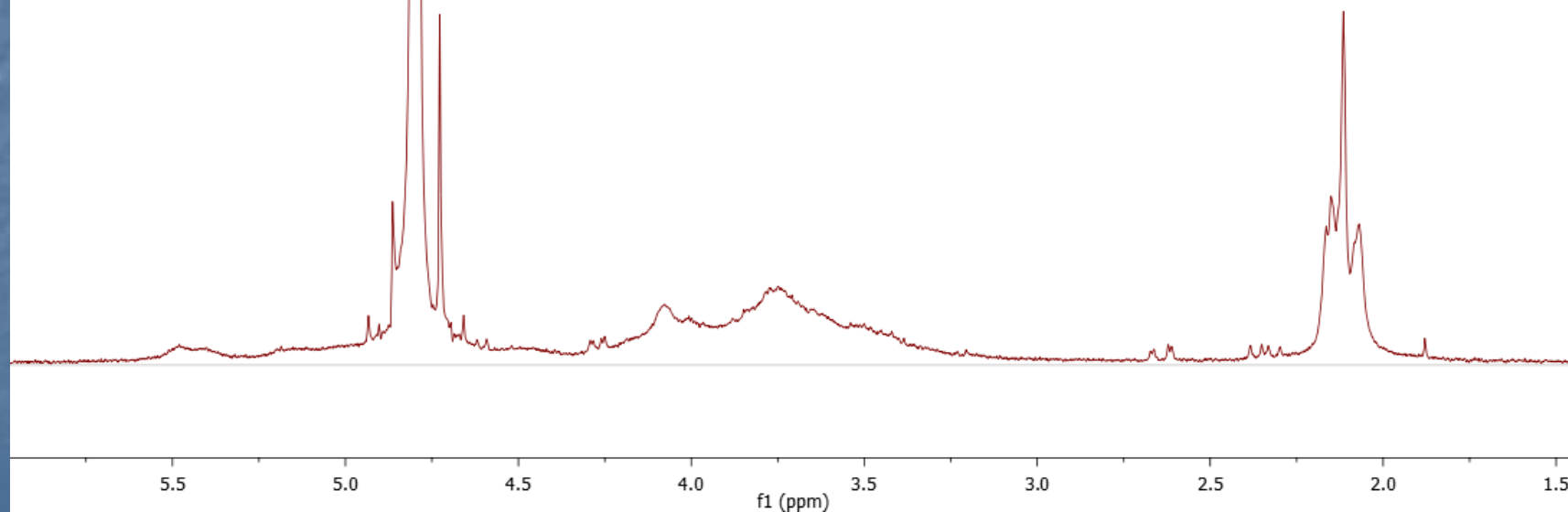
Aloe Vera Inner Leaf Juice Constituents and Additives that need to be Analyzed and Reported for IASC Certification

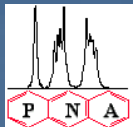
Compound	IASC Certification requirement
Acemannan	$\geq 5\%$ dry weight
Acetylated PS	
Glucose	Present
Aloin	10 ppm or less in 0.5% aloe vera solids solution, analysed by HPLC or other fit for purpose methodology approved by IASC
Isocitrate	$\leq 5\%$ dry weight
Maltodextrin	Must be listed on label and analysis must meet label claims. If undeclared, is considered an adulterant.
Solids	$\geq 0.46\%$ in single-strength juice (for example, a 10x concentrate should have $\geq 4.6\%$)
Ash	$\leq 40\%$

Acetylated Polysaccharide 90%+



Scheme 1: Proposed structure for the major component of *Aloe vera* polysaccharide





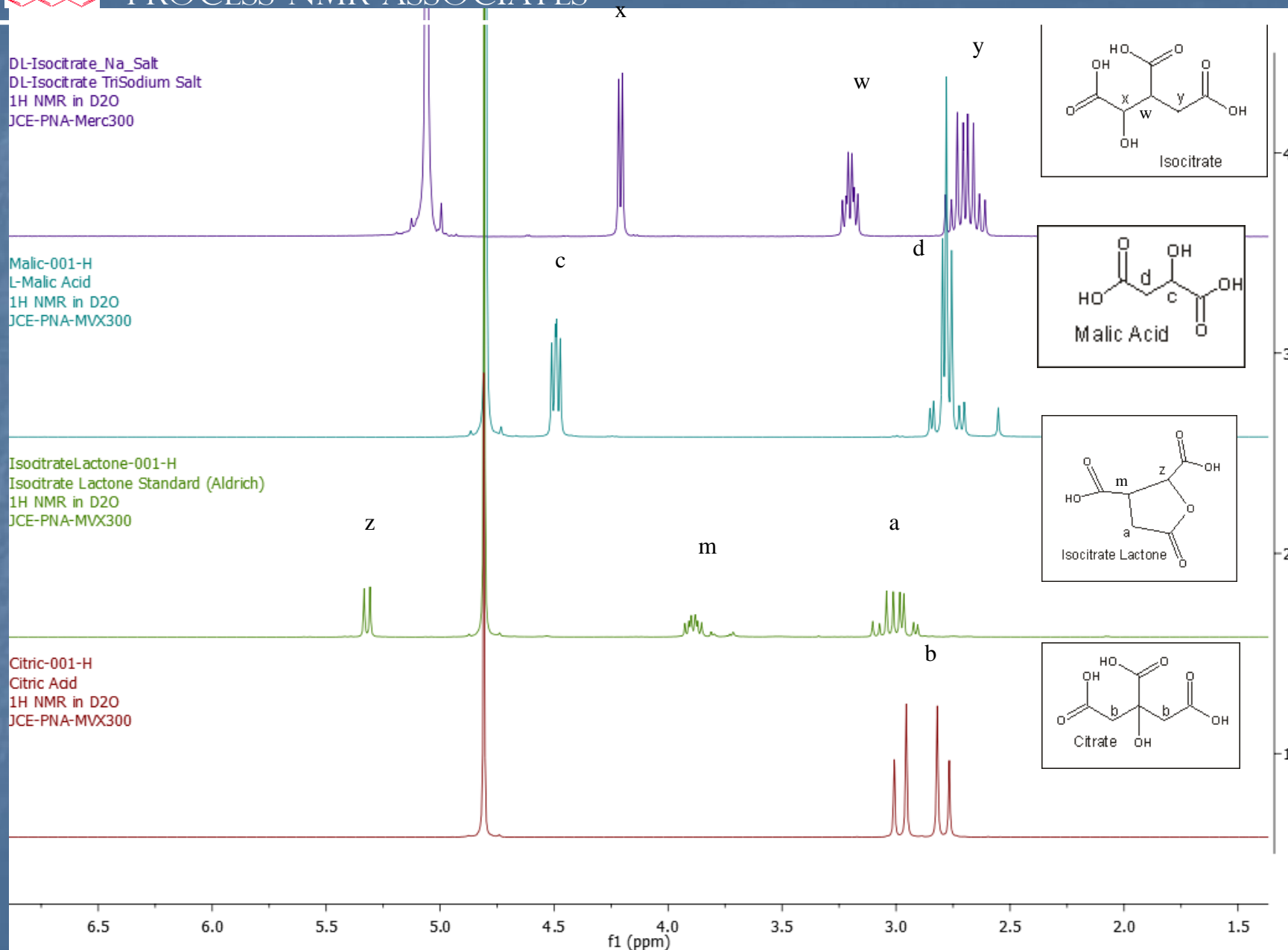
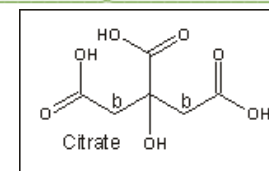
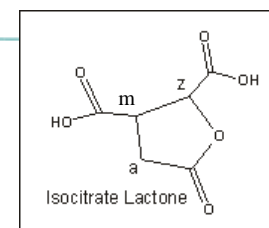
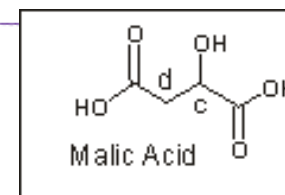
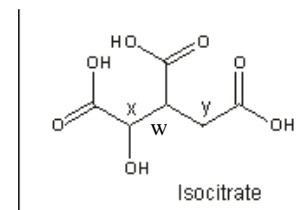
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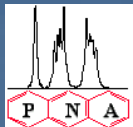
DL-Isocitrate_Na_Salt
DL-Isocitrate TriSodium Salt
1H NMR in D2O
JCE-PNA-Merc300

Malic-001-H
L-Malic Acid
1H NMR in D2O
JCE-PNA-MVX300

IsocitrateLactone-001-H
Isocitrate Lactone Standard (Aldrich)
1H NMR in D2O
JCE-PNA-MVX300

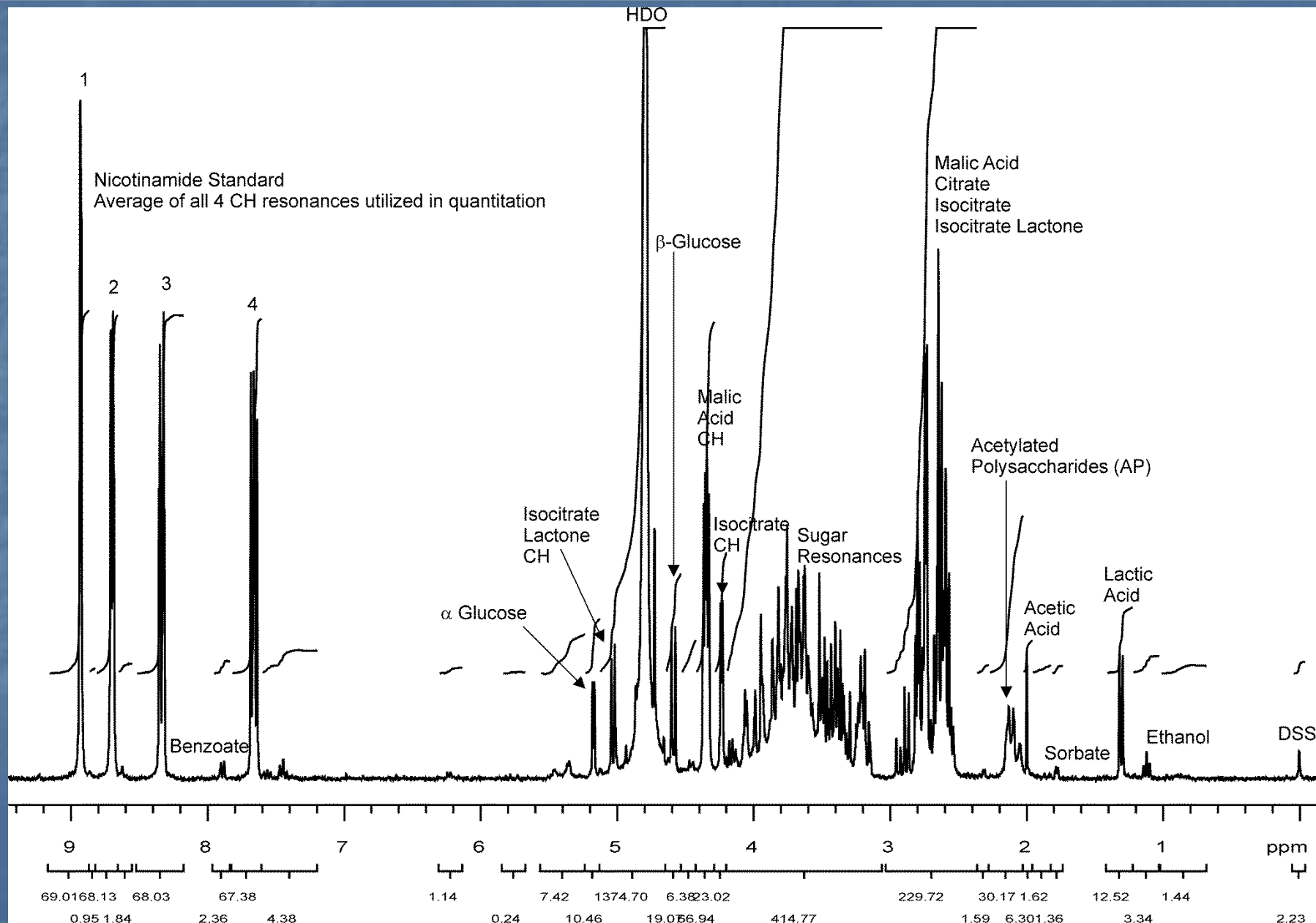
Citric-001-H
Citric Acid
1H NMR in D2O
JCE-PNA-MVX300

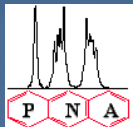




Commercial freeze-dried 200x aloe vera leaf juice powder

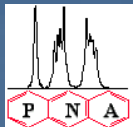
PROCESS NMR ASSOCIATES



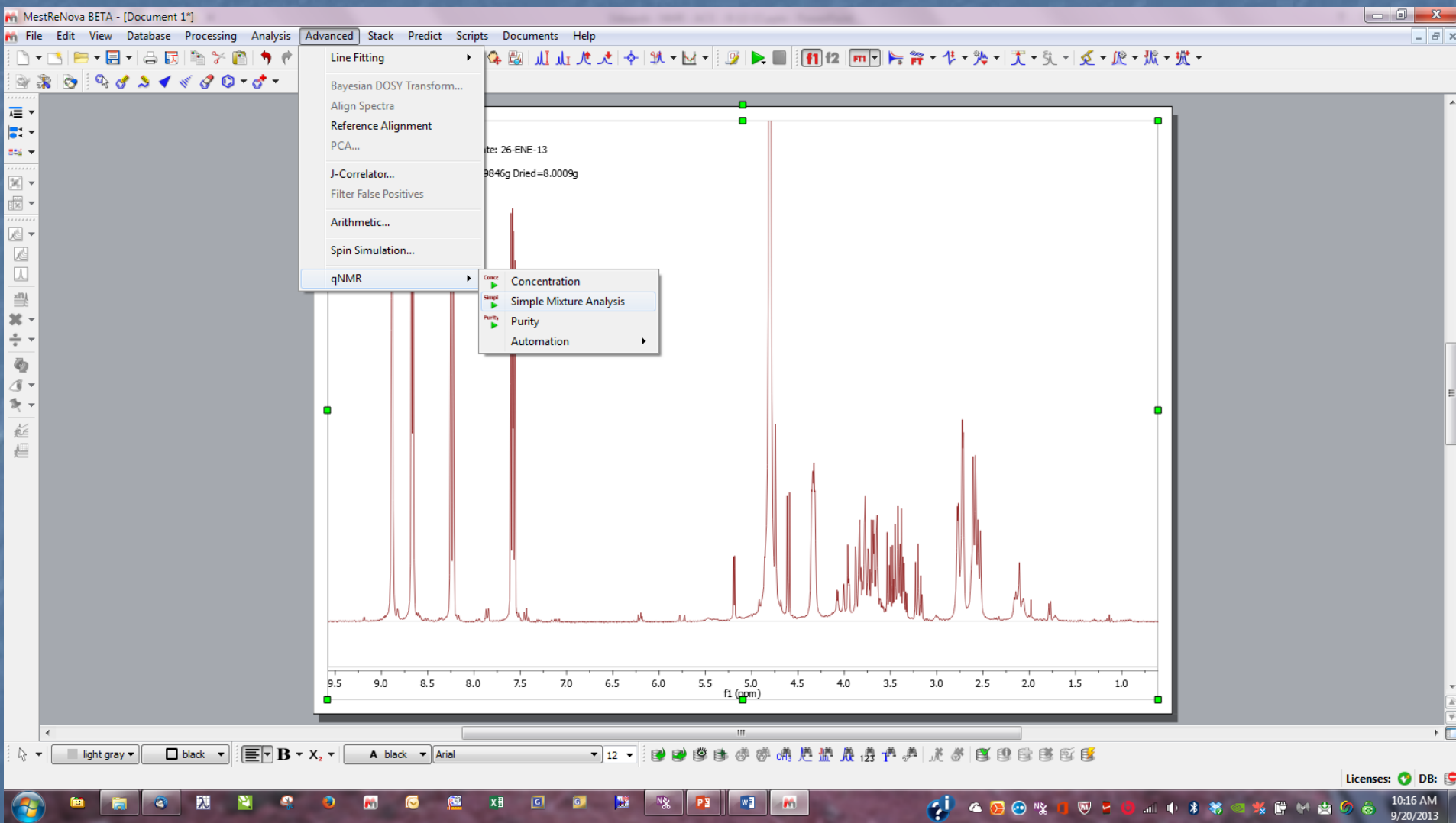


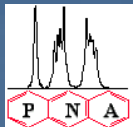
Chemical shift values, peak and chemistry descriptions, molar conversion factors that can be used for detection and quantitation of aloe vera leaf juice preservatives, additives, and degradation products

Compound	Type of compound	Signal type	Chemical shift, ppm
Propylene glycol	Additive	CH ₃ , doublet (N=3)	1.1
Ethanol	Degradation product or additive	CH ₃ , triplet (N=3)	1.15
Lactic acid	Degradation product	CH ₃ , doublet (N=3)	1.33
Potassium sorbate	Preservative	CH ₃ , doublet (N=3)	1.82
Acetic acid	Degradation product	CH ₃ , singlet (N=3)	1.96
Pyruvic acid	Degradation product	CH ₃ , singlet (N=3)	2.35
Citric acid	Naturally present or added as pH regulator or preservative	2 x CH ₂ , Multiplet (N=4)	2.5-3.0
Succinic acid	Degradation product	2 x CH ₂ , singlet (N=4)	2.6
Glycerol	Additive	CH ₂ and CH, multiplet	3.5
Glycine	Additive	CH ₂ , singlet (N=2)	3.51
Sucrose	Additive	CH, doublet (N=1)	5.4
Fumaric acid	Degradation product	2 x CH, singlet (N=2)	6.5
Sodium benzoate	Preservative	2 x CH, doublet (N=2)	7.95
Formic acid	Degradation product	CH, singlet (N=1)	8.2-8.3

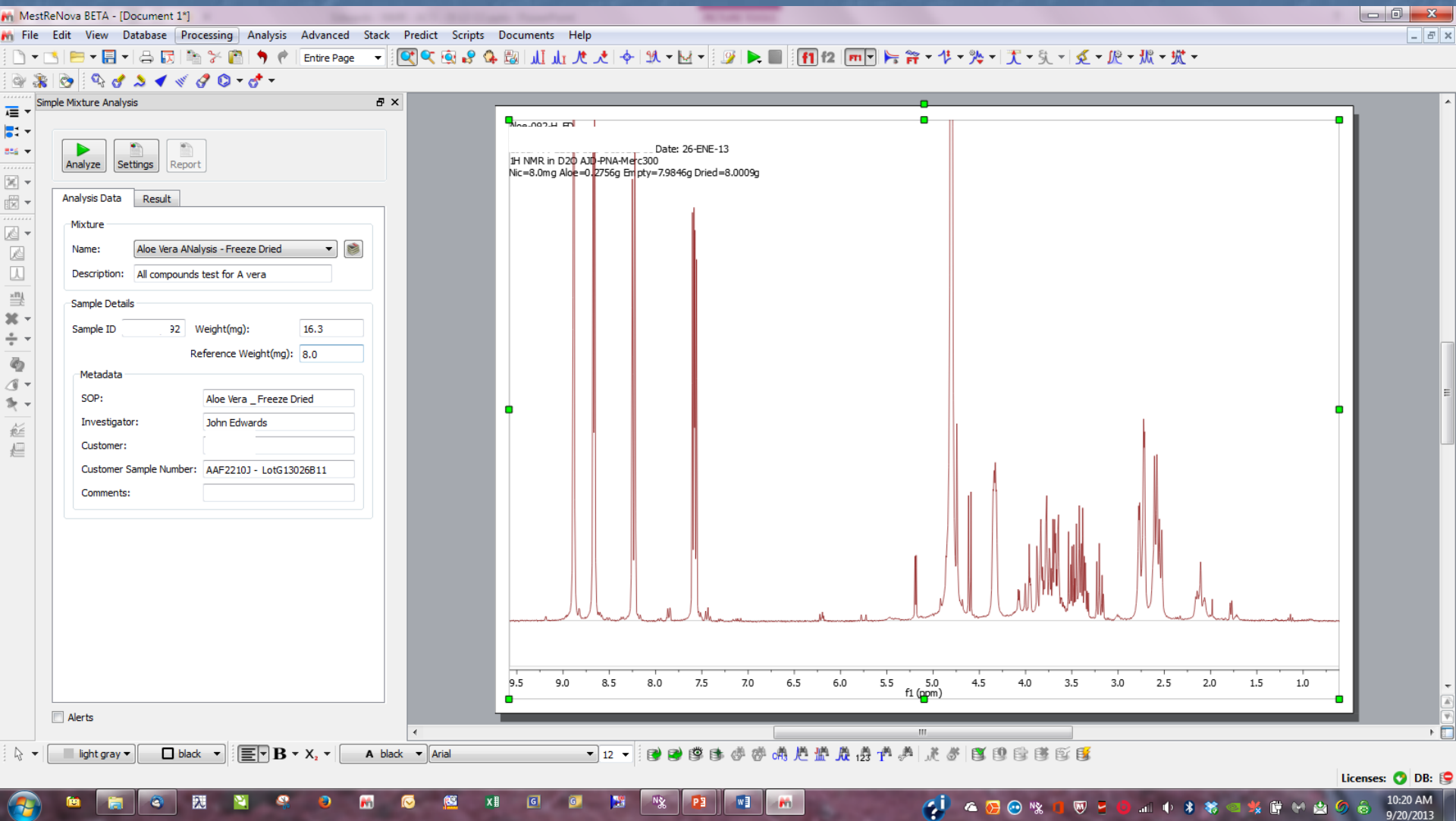


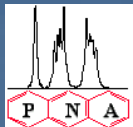
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MestReNova BETA - [Document 1*]

File Edit View Database Processing Analysis Advanced Stack Predict Scripts Documents Help

Entire Page

Simple Mixture Analysis

Analyze Settings Report

Analysis Data Result

Mixture

Name: Aloe Vera ANALYSIS - Freeze Dried

Description: All compounds test for A vera

Sample Details

Sample ID: Weight(mg): 16.3

Reference Weight(mg): 8.0

Metadata

SOP: Aloe Vera _ Freeze Dried

Investigator: John Edwards

Customer:

Customer Sample Number: AAF2210J - LotG13026B11

Comments:

Alerts

Library

Current Library: D:\MNOVA\A. vera test 1

Experiment	Description
1 A vera 1	All compounds test for A vera
2 Aloe Vera ANALYSIS - Freeze Dried	All compounds test for A vera
3 Aloe - Acid - Maltodextrin - WL	All compounds test for A vera
4 t5	All compounds test

OK Cancel

111 Date: 26-ENE-13

¹H NMR in D₂O A10-PNA-Merc300

Nic=8.0mg Aloe=0.2756g Empty=7.9846g Dried=8.0009g

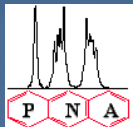
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0

f1 (ppm)

light gray black B X₂ A black Arial 12

Licenses: DB:

10:22 AM 9/20/2013



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MestReNova BETA - [Document 1*]

File Edit View Database Processing Analysis Advanced Stack Predict Scripts Documents Help

Entire Page

Simple Mixture Analysis

Analyze Settings Report

Analysis Data Result

Mixture

Name: Aloe Vera Analysis - Freeze Dried

Description: All compounds test for A vera

Sample Details

Sample ID: 92 Weight(mg): Reference Weight(mg)

Metadata

SOP: Aloe Vera _ Freeze

Investigator: John Edwards

Customer:

Customer Sample Number: AAF22101 - LotG1

Comments:

Alerts

Experiment

Experiment Name: Aloe Vera Analysis - Freeze Dried

Description: All compounds test for A vera

Compound	Type	Mol. Weight	Color	Spectrum
acetic a	Compound	60.05	Blue	1
gluc	Compound	180.16	Blue	1
Isocitric a	Compound	192.12	Blue	1
isocitric lactone	Compound	174.11	Blue	1

Compound Editor

Name: malic a

Color: Blue Spectrum N°: 1 Molecular Weight: 134.09

Type: Compound Acceptable Limit From: 1 To: 20

Formula: $100 \cdot (RW \cdot I^1 \cdot NN \cdot MW) / (IR \cdot I^1 \cdot NN \cdot MW \cdot S \cdot W)$

Ranges

	From	To	NN
1	4.38	4.27	1

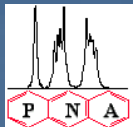
OK Cancel

OK Cancel

5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 (ppm)

light gray black B X₂ A black Arial 12

Licenses: DB: 10:24 AM 9/20/2013



PROCESS NMR ASSOCIATES

MestReNova BETA - [Document 1*]

File Edit View Database Processing Analysis Advanced Stack Predict Scripts Documents Help

Entire Page

Simple Mixture Analysis

Analyze Settings Report

Analysis Data Result

Mixture

Name: Aloe Vera ANALYSIS - Freeze Dried

Description: All compounds test for A vera

Sample Details

Sample ID: . Weight(mg):

Reference Weight(mg):

Metadata

SOP: Aloe Vera _ Freeze

Investigator: John Edwards

Customer: 3

Customer Sample Number: AAF2210J - LotG1

Comments:

Alerts

Experiment

Experiment Name: Aloe Vera ANALYSIS - Freeze Dried

All compounds test for A vera

Formula Editor

$$100 * (RW * I1 * NNR1 * MW) / (IR1 * NN1 * MWR * SW)$$

Check Formula

LEGEND:

CONCENTRATIONS OF OTHER COMPOUNDS:

C1: Concentration of: lactic a

C2: Concentration of: b gluc

C3: Concentration of: a gluc

CCF : Concentration Factor of Reference

C5: Concentration of: AP

C6: Concentration of: acetic a

C7: Concentration of: gluc

C8: Concentration of: Isocitric a

C9: Concentration of: isocitric lactone

C10: Concentration of: Ethanol

INTEGRALS:

IR1: Reference Integral of range [7.66 , 7.55]

I1: Integral of range [4.38 , 4.27]

NUMBER OF NUCLIDES:

NNR1: Reference Nucleides of range [7.66 , 7.55]

NN1: Nucleides of range [4.38 , 4.27]

OTHERS:

MW: Molecular Weight

SW: Sample Weight

RW: Reference Weight

MWR : Molecular Weight of Reference

OK Cancel

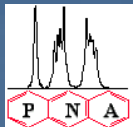
OK Cancel

5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0

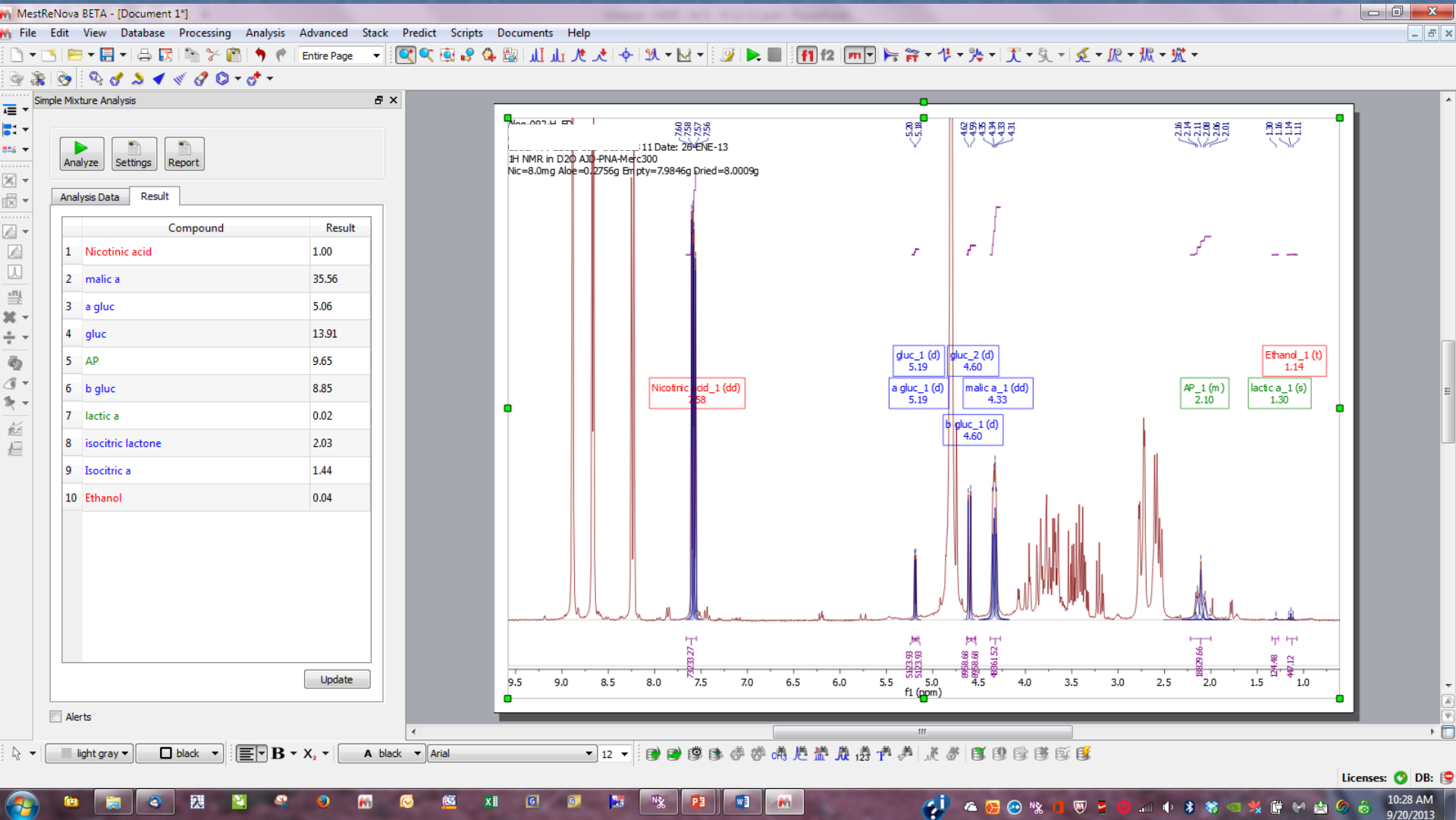
light gray black B X A black Arial 12

Licenses: DB:

10:25 AM 9/20/2013



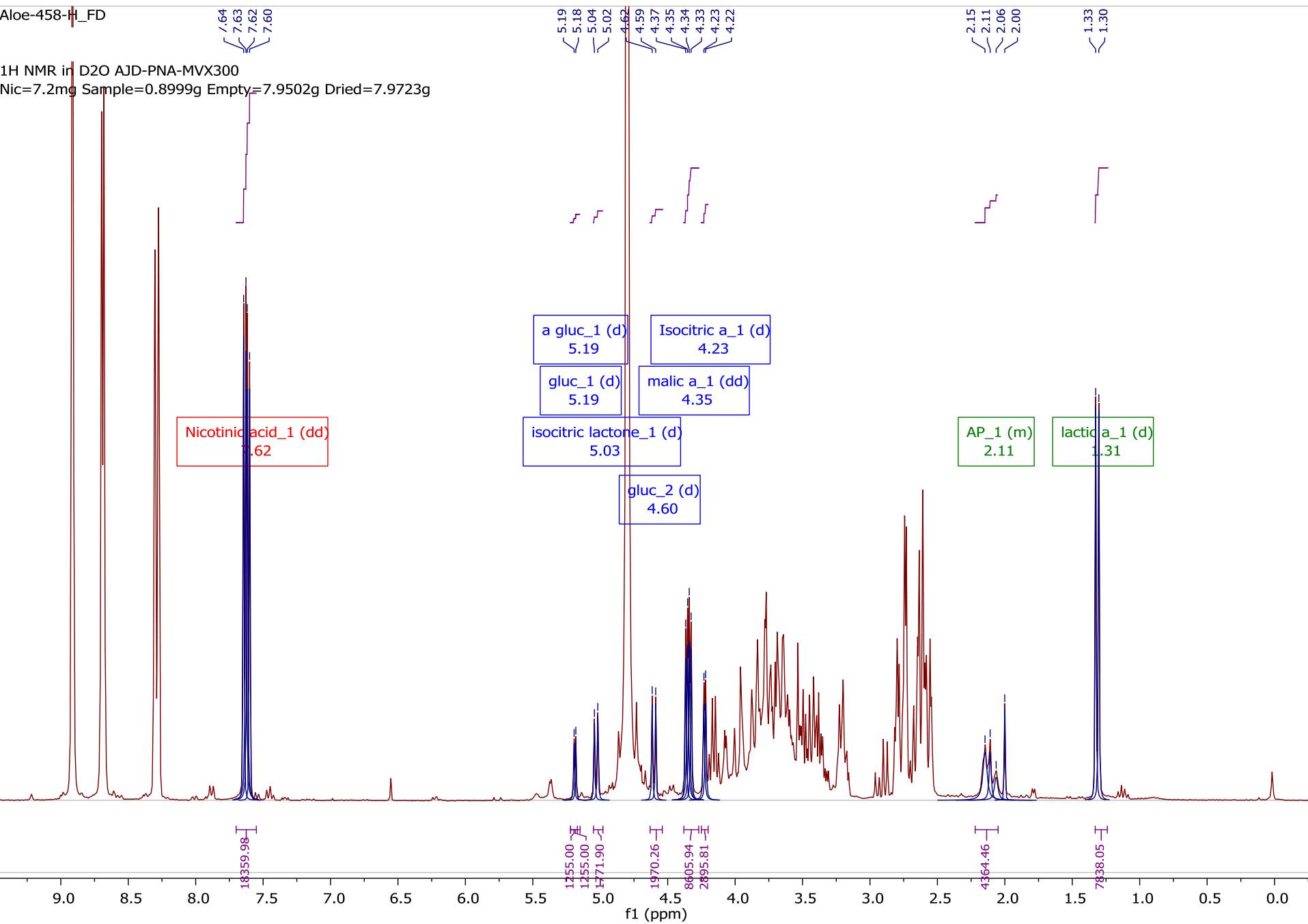
PROCESS NMR ASSOCIATES

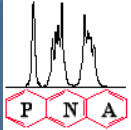


Aloe-458-H_FD

¹H NMR in D₂O AJD-PNA-MVX300

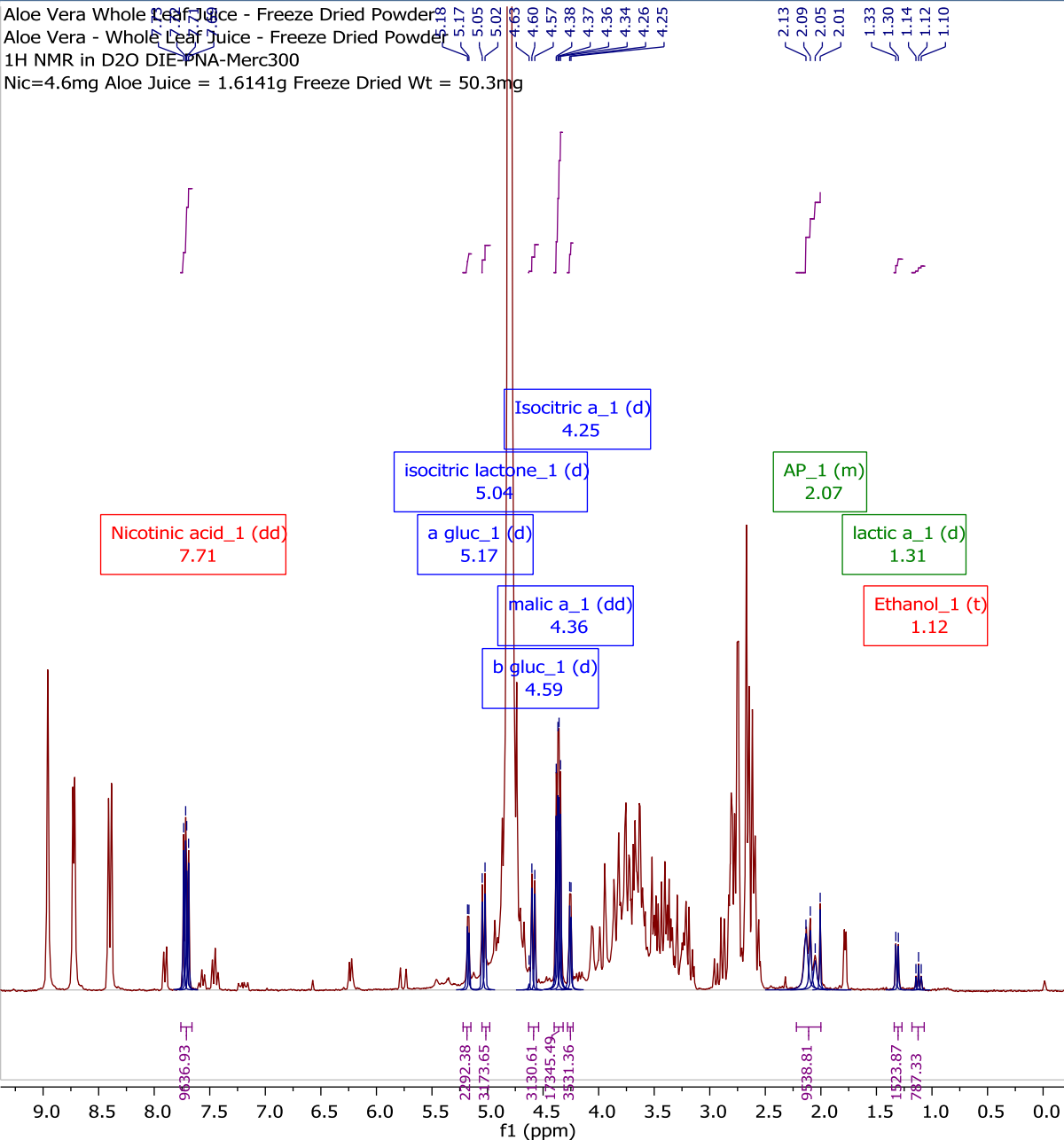
Nic=7.2mg Sample=0.8999g Empty=7.9502g Dried=7.9723g





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Aloe Vera Whole Leaf Juice - Freeze Dried Powder
Aloe Vera - Whole Leaf Juice - Freeze Dried Powder
1H NMR in D2O DIE-PNA-Merc300
Nic=4.6mg Aloe Juice = 1.6141g Freeze Dried Wt = 50.3mg



Compound	Concentration
Nicotinic acid	1.00
lactic a	0.36
a gluc	3.21
isocitric lactone	4.29
malic a	18.06
Isocitric a	5.27
b gluc	4.38
AP	6.92
acetic a	0.06
Ethanol	0.09

Sample Details:

Sample ID: AVWL-92

Sample Weight: 50.3

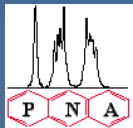
Reference Weight: 4.6

SOP: Aloe Vera _ Freeze Dried

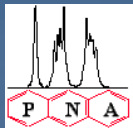
Investigator: John Edwards

Customer: Aloe

Customer Sample Number: 1x WL



2) Pre-Processing of Large NMR Datasets for Chemometric Regression Analyses to Derive Chemical and Physical Properties



Third Generation NMR - 2013– Aspect AI NMR System

New magnet design – 30mm bore size

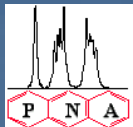
- The amount of magnetic pieces that assemble the magnet reduced from 34 to 10. Reduction in Mechanical Complexity
- Bore size of the magnet was increased to 30 mm - improved temperature susceptibility
- Improved temperature and shim stability.

New Digital Spectrometer Design - reduces footprint, improves signal processing capabilities

Probe - Improved Probe Q for Higher Sensitivity.

Software – Windows 7 – Improved Chemometric Capabilities





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September 12, 2013



42 MHz NMR
3-5 mm Samples
Lab Only



60 MHz NMR
3-5 mm Samples
Lab Only



60 MHz NMR
3-5 mm Samples
Lab Only



MobiLab™ SPECTRA 2T

85+ MHz NMR
3-5 mm Samples
Lab Only

nanalysis

NMReady 60

60 MHz NMR
3-5 mm Samples
Lab Only



Picospin 45 and 80

45 MHz and 82 MHz NMR
300 micron capillary injection
Lab Only

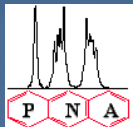


60 MHz NMR
3-10 mm Samples
Lab or On-Line

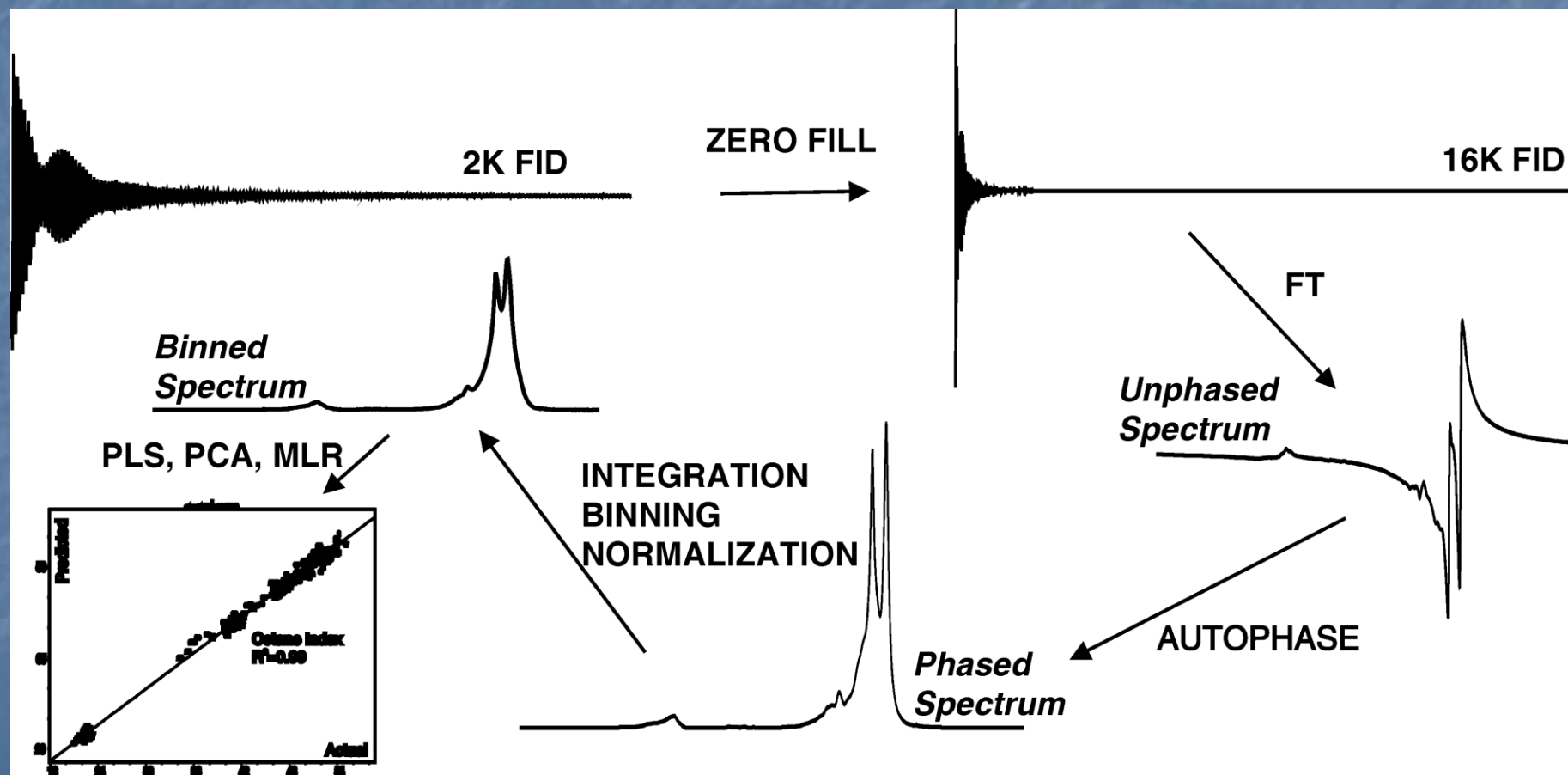


aspectimaging

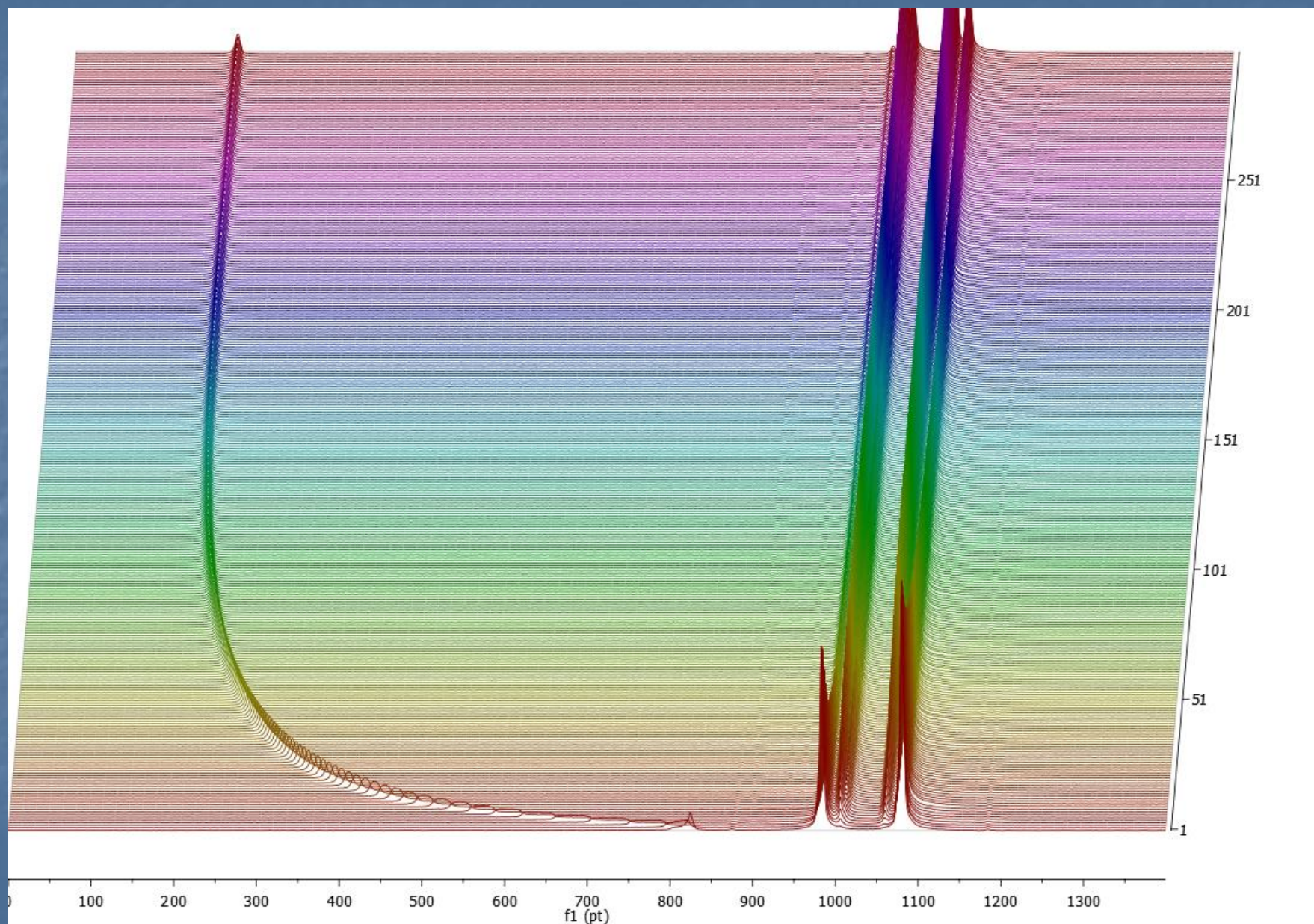
60 MHz NMR
3-10 mm Samples
Lab or On-Line

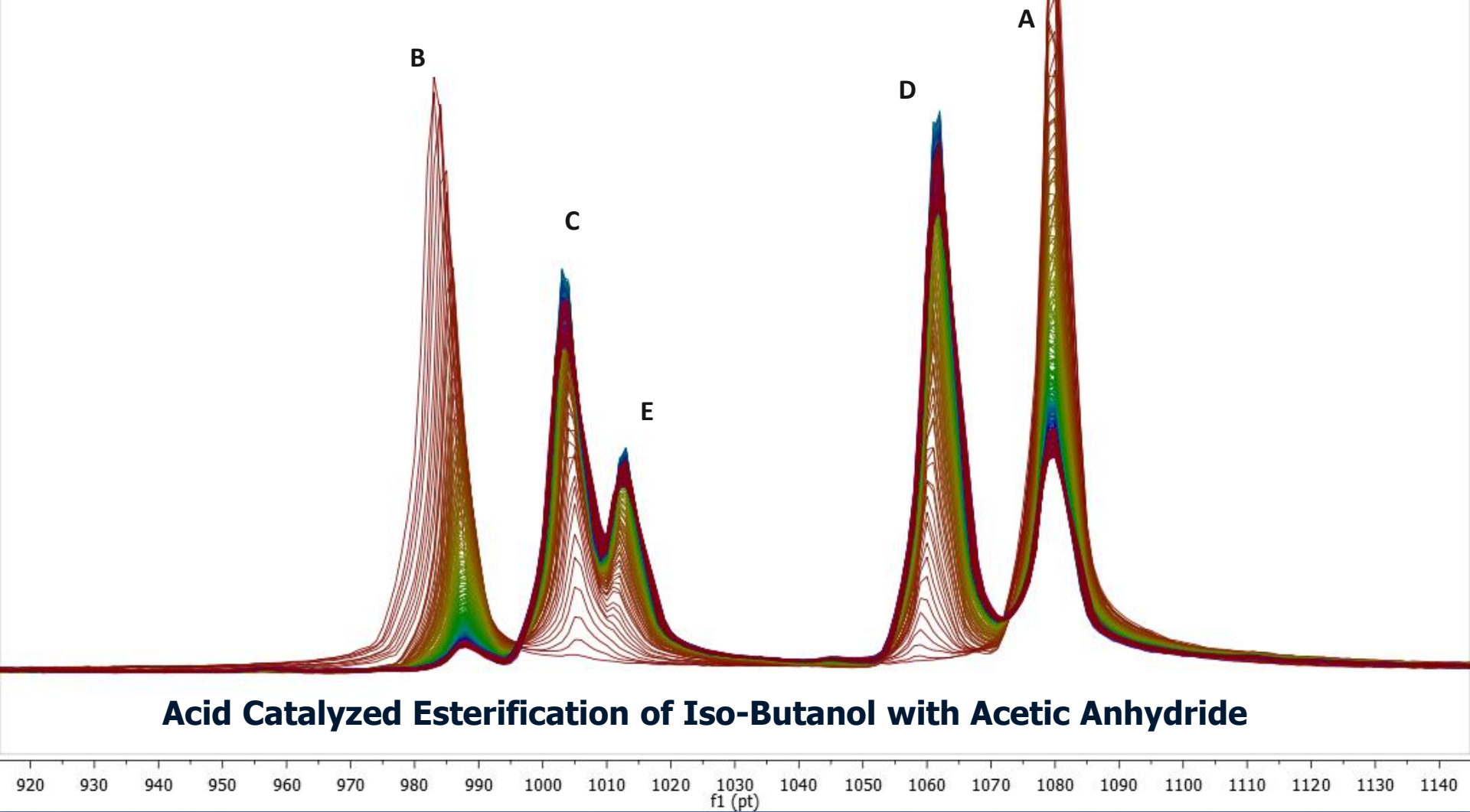
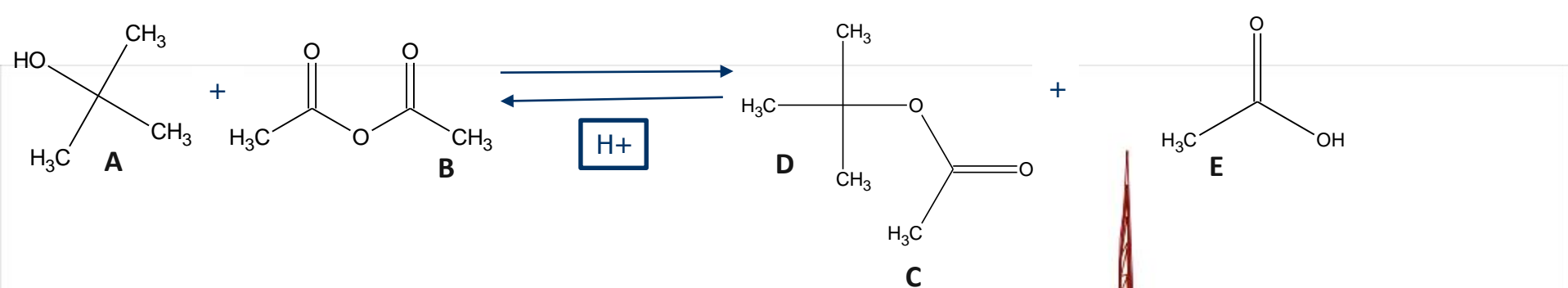


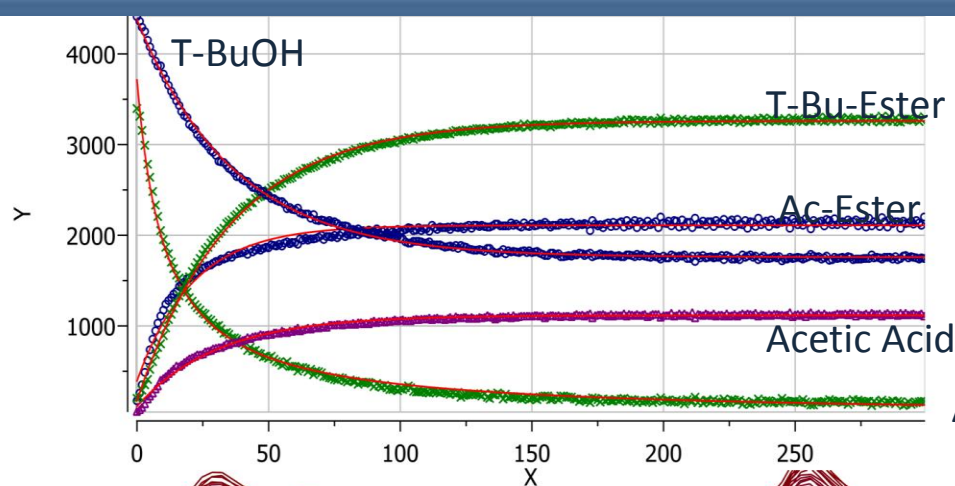
NMR Data Processing for Input into Chemometrics – PCA/PLS



^1H NMR Reaction Monitoring – Esterification of t-butanol with acetic anhydride



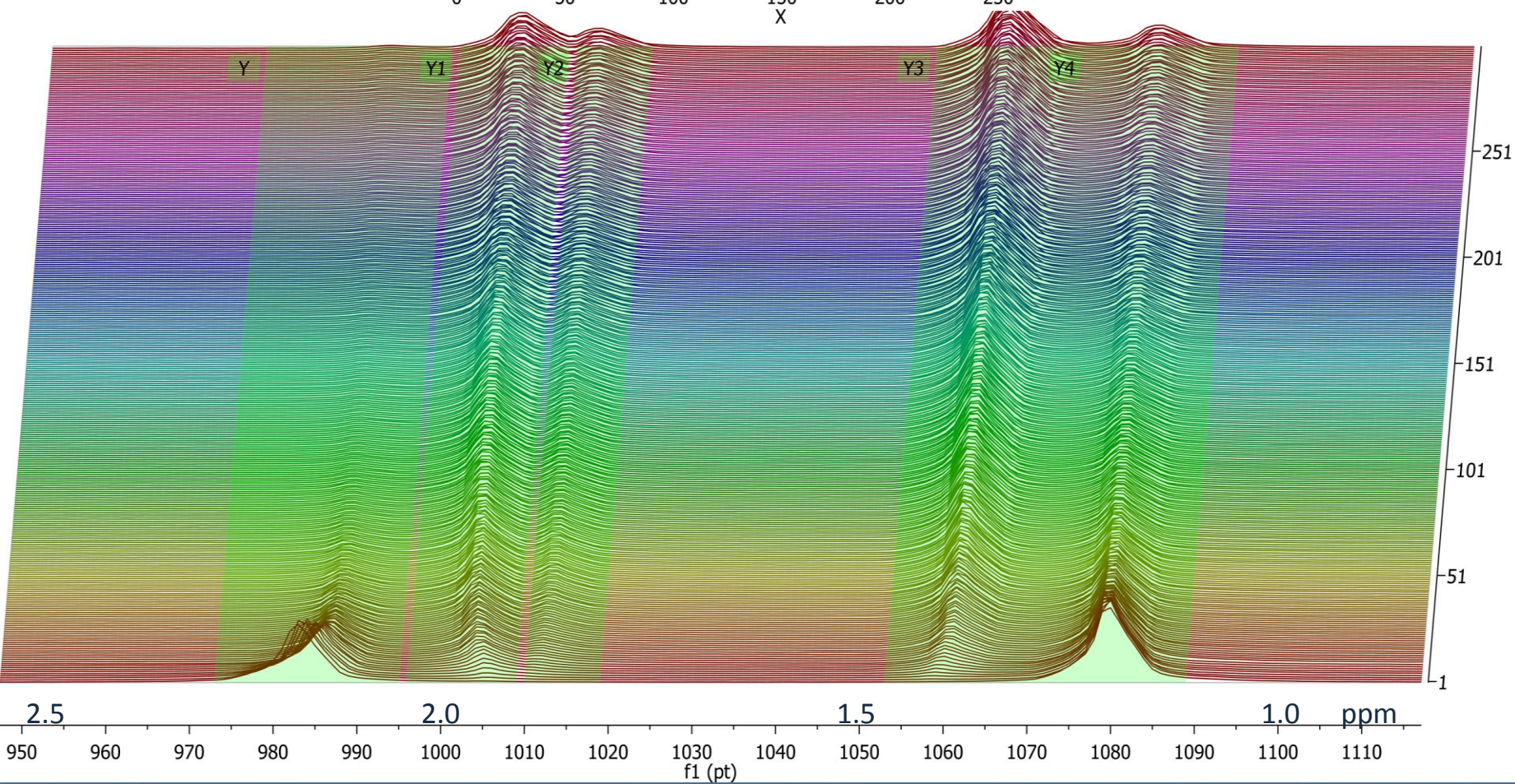




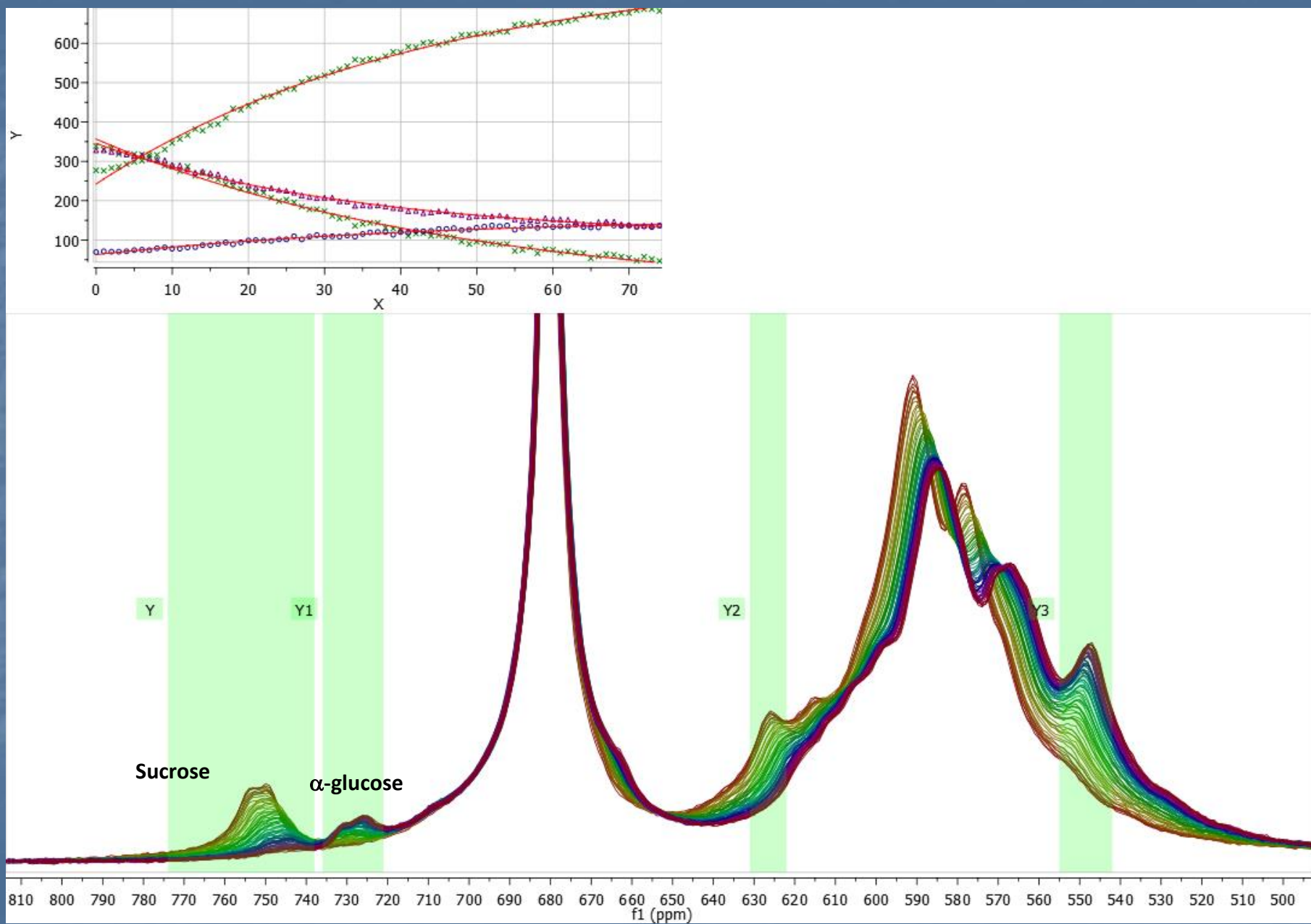
Esterification of t-BuOH

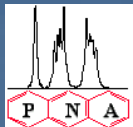
Integral Graph
And Integration Plot

AcAn

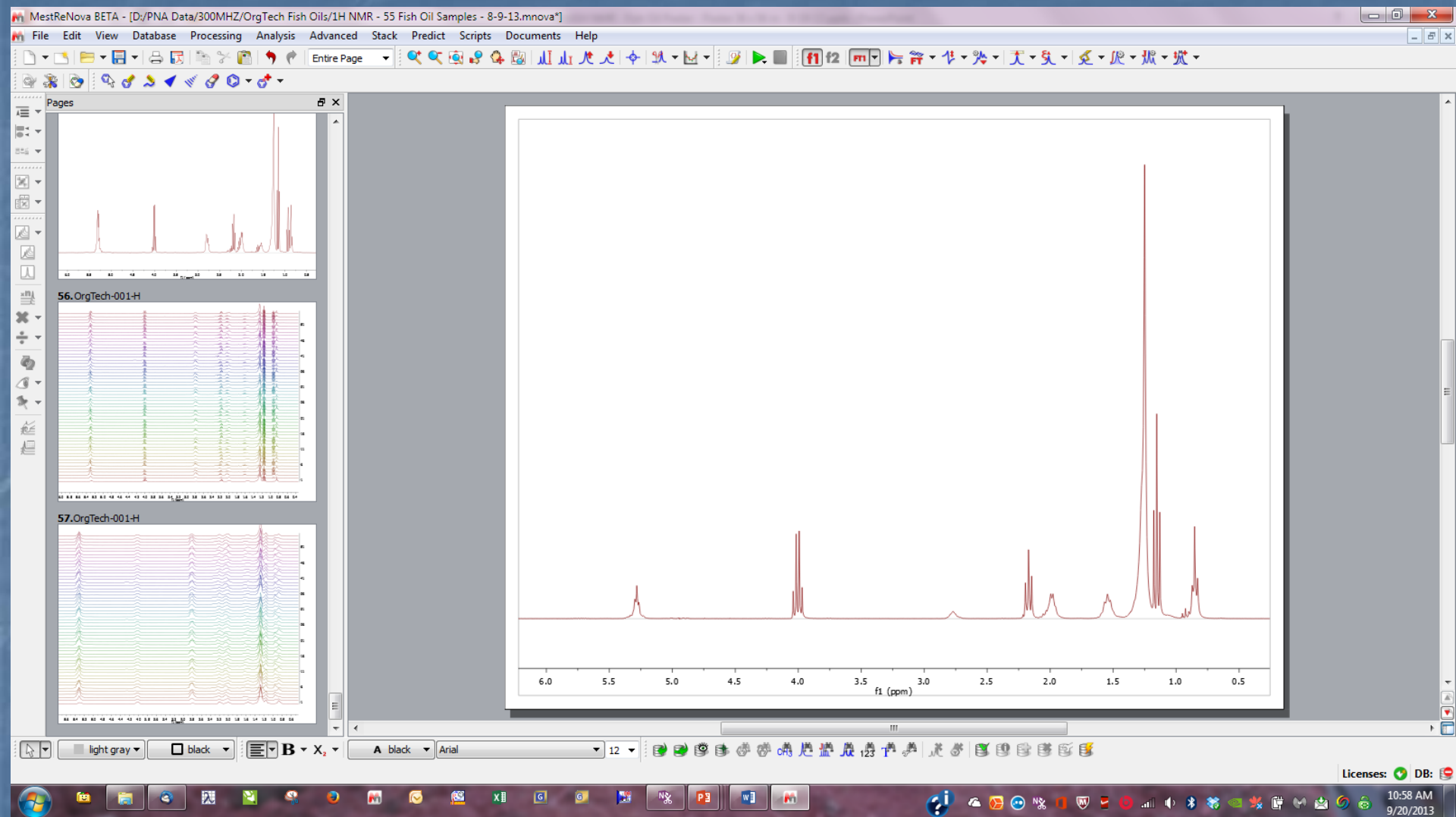


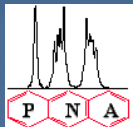
1H NMR – Sucrose Hydrolysis by Invertase Enzyme



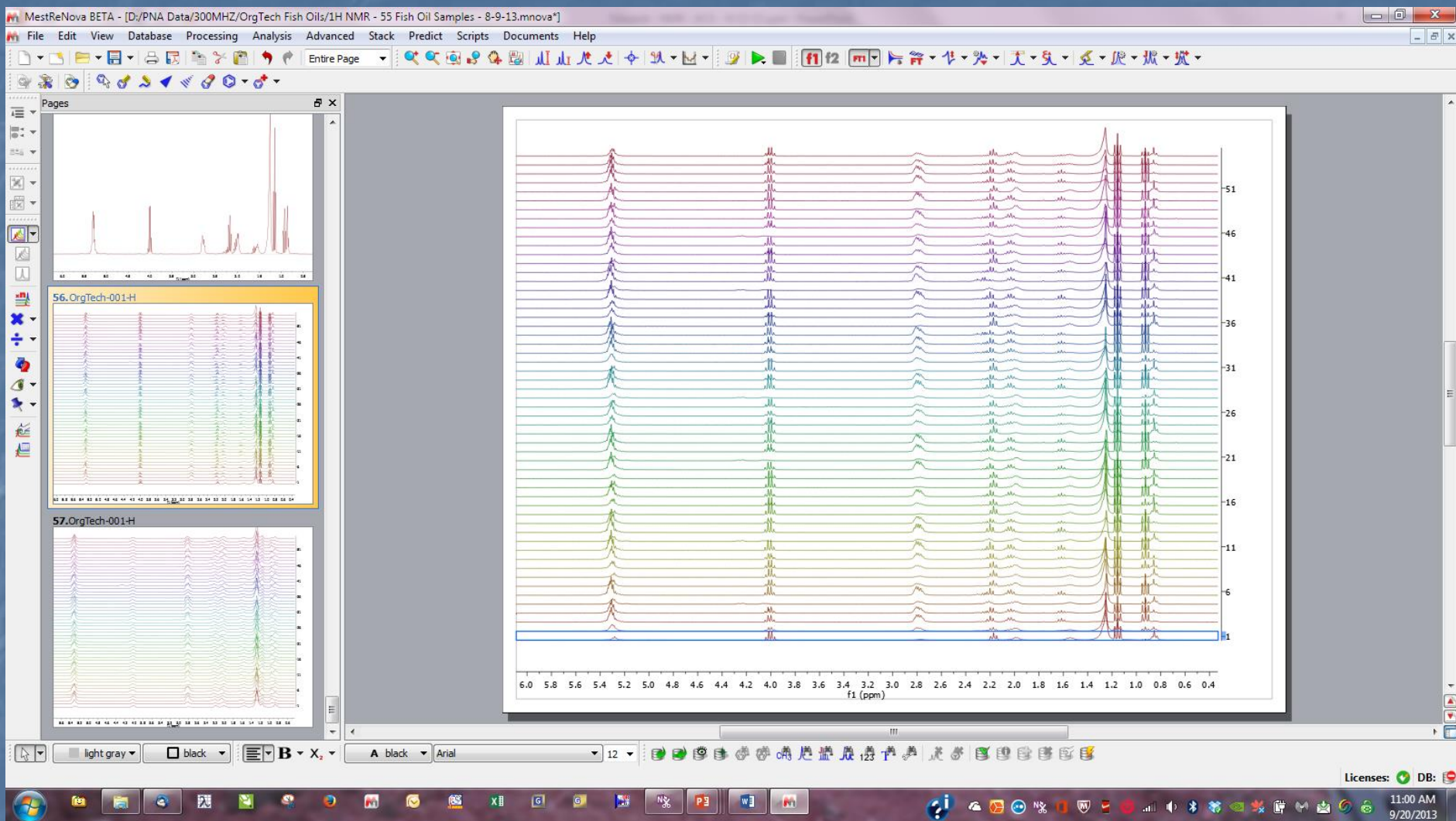


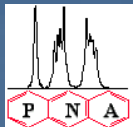
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MestReNova BETA - [D:\PNA Data\300MHZ\OrgTech Fish Oils\1H NMR - 55 Fish Oil Samples - 8-9-13.mnova*]

File Edit View Database Processing Analysis Advanced Stack Predict Scripts Documents Help

Processing Template...

Recent Processing Templates

Break Processing On

Group Delay...

FID Shift...

Diagonal Suppression...

Signal Suppression...

Drift Correction...

Apodization...

Truncate...

Zero Filling and LP...

Fourier Transform...

Symmetrize

Tilt 45

Reduce t1 Noise

Covariance NMR

Normalize...

Binning

Compression...

Smoothing...

Resolution Booster...

Reference Deconvolution...

Invert

Transpose

Set Processing Dimension

Phase Correction

Baseline

Reverse Spectrum

Regular Binning...

Variable Binning...

GSD Binning...

Regular Binning

Apply To

☐ Full Spectrum

From: 0.44 ppm

To: 5.80 ppm

Width of Each Integral Region

0.040000 ppm

Method

Average Sum

☐ Save

C:\Users\John\binning.csv

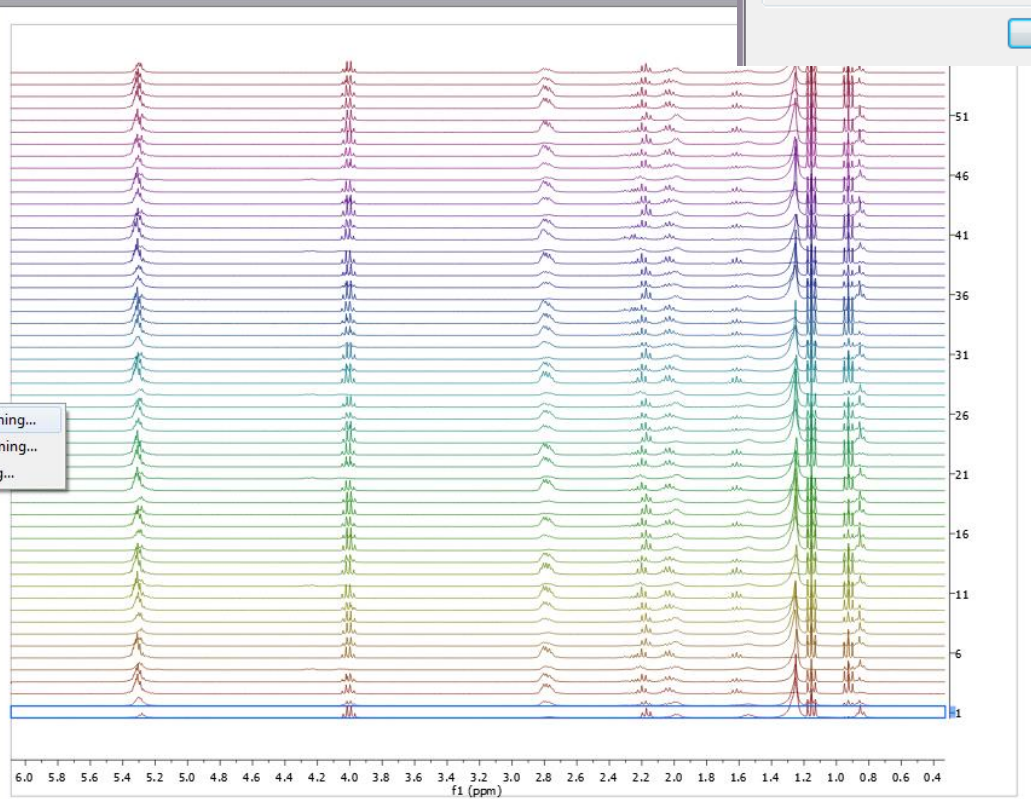
Tip

Use **Cuts** view command if you want to exclude any regions (such as water region).

Include **Class** definition into Stacked Spectra Table.

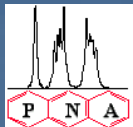
OK

Cancel



Licenses: DB:

11:01 AM
9/20/2013



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MestReNova BETA - [D:\PNA Data\300MHz\OrgTech Fish Oils\1H NMR - 55 Fish Oil Samples - 8-9-13.mnova*]

Save As

Organize New folder

File name: 1H NMR - 55 Fish Oil Samples - 8-9-13

Save as type: MestReNova Document (*.mnova)

MestReNova Document (*.mnova)

MestReNova Pages (*.mnpag)

MestReNova Customization (*.mncs)

Adobe PDF Files (*.pdf)

BMP Image (*.bmp)

Encapsulated PostScript (*.eps)

Enhanced Metafile (*.emf)

Galactic (*.spc)

JCAMP-DX (*.jcamp *.dx *.jdx *.jcm)

JPEG Image (*.jpeg)

MestReC (*.mrc)

NMR CSV File (*.csv *.txt)

PNG Image (*.png)

PPM Image (*.ppm)

PostScript (*.ps)

SVG Image (*.svg)

TIFF Image (*.tiff)

XBM Image (*.xbm)

XPM Image (*.xpm)

Script: NMR 1D Custom CSV (*.csv *.txt)

Script: NMR CSV Matrix (*.csv *.txt)

Script: NMR CSV Matrix (Transposed) (*.csv *.txt)

57.OrgTech-054

light gray

black

B X

A black Arial

12

Help

f1 f2 m

1H NMR - 55 Fish Oil Samples - 8-9-13

1H NMR - 55 Fish Oil Samples - Processed - 8-9

1H NMR - 55 Fish Oil Samples - Processed - 8-9

13C NMR Data - 0.05 ppm

13C NMR Data - 0.5 ppm

13C NMR Data - Total

Predictions EPA DHA

Help

f1 f2 m

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1H NMR - 55 Fish Oil Samples - Processed - 8-9

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13C NMR Data - 0.5 ppm

13C NMR Data - Total

Predictions EPA DHA

57.OrgTech-054

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B X

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12

Help

f1 f2 m

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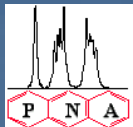
12

Help

f1 f2 m

1H NMR - 55 Fish Oil Samples - 8-9-13

1H NMR - 55 Fish Oil Samples - Processed - 8-9



Transposed CSV Output of Stacked Plot – Yields rows that have integration bin values

Input as X Variable Data into Chemometrics Software Packages

1H NMR - 55 Fish Oil Samples - Processed - 8-9-13 - Transposed.txt - Excel

FILEHOMEINSERTPAGE LAYOUTFORMULASDATAVIEWREVIEWVIEWADD-INS

Team

Sign in

CutCopyFormat Painter

Paste

Clipboard

Calibri11

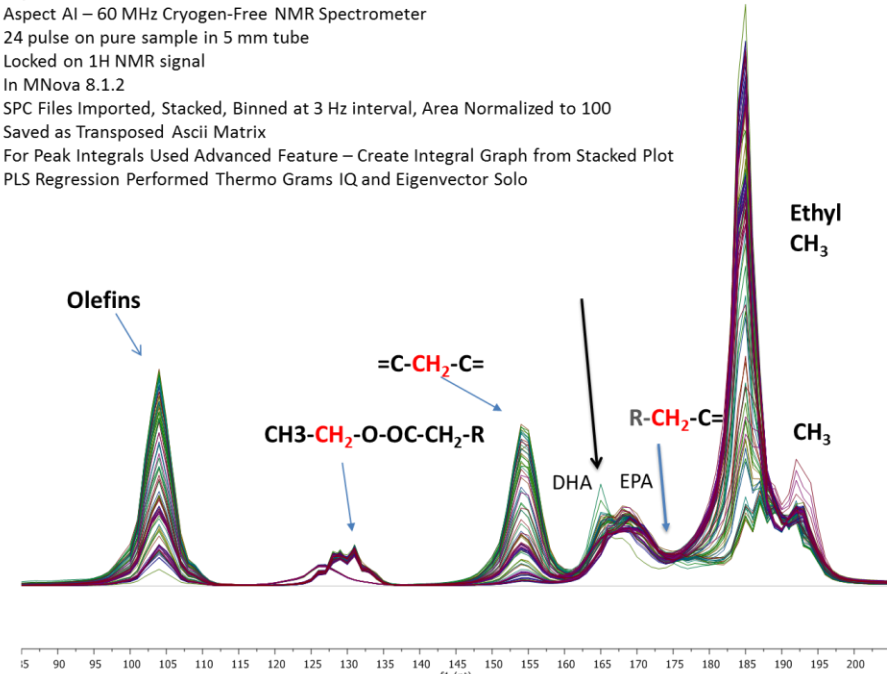
<

PLS Regression Analysis to Obtain Predictive Model of EPA and DHA Omega-3 Fatty Acids at Various Points Of Nutritional Supplement Manufacturing Process

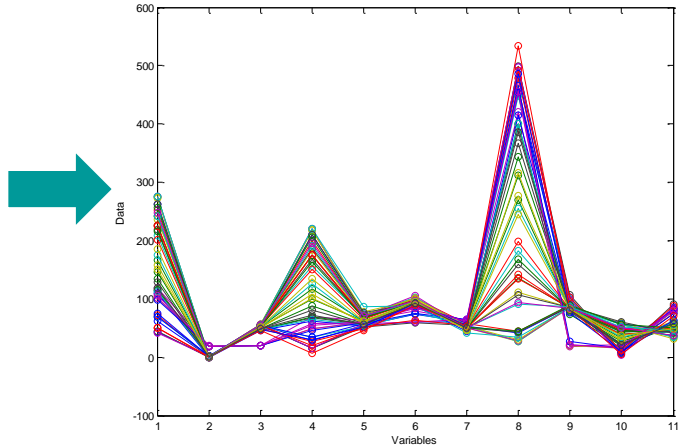
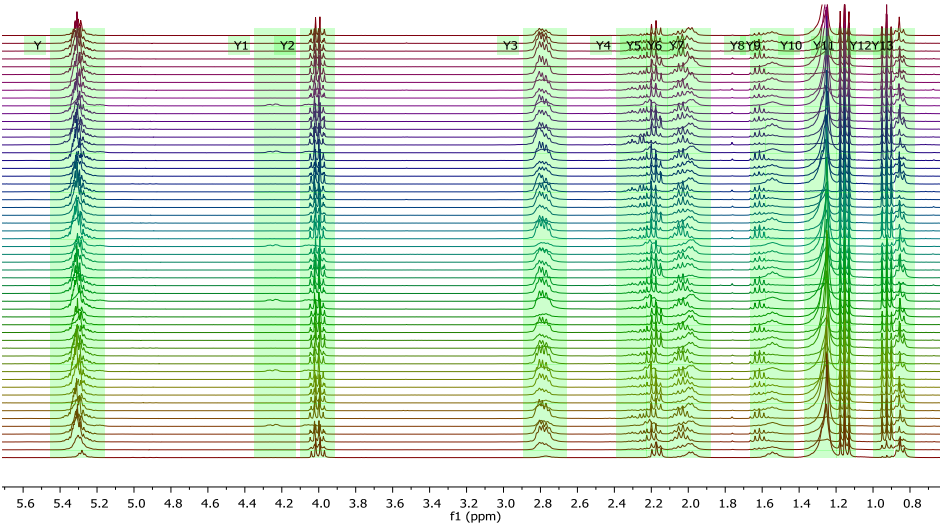
¹H NMR – 60 MHz

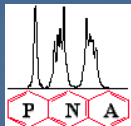
Experimental

Aspect AI – 60 MHz Cryogen-Free NMR Spectrometer
24 pulse on pure sample in 5 mm tube
Locked on ¹H NMR signal
In MNova 8.1.2
SPC Files Imported, Stacked, Binned at 3 Hz interval, Area Normalized to 100
Saved as Transposed Ascii Matrix
For Peak Integrals Used Advanced Feature – Create Integral Graph from Stacked Plot
PLS Regression Performed Thermo Grams IQ and Eigenvector Solo



NMR ID	EPA (Area %)	DHA (Area %)	Sample Description
FO3h001	0.64	0.01	First Esterification
FO3h002	21.55	13.34	First Esterification
FO3h003	62.97	15.66	Clathration
FO3h004	29.43	18.16	Mol Dist
FO3h005	14.21	9.54	Pollock Oil
FO3h006	52.74	28.90	Separator
FO3h007	15.21	10.51	PolyUnsat Ester
FO3h008	7.18	0.23	First Esterification
FO3h009	16.95	10.04	First Esterification
FO3h010	36.35	16.47	Clathration
FO3h011	61.09	21.26	Mol Dist
FO3h012	13.32	5.95	MSC Pollock Oil
FO3h013	71.78	7.43	Separator
FO3h014	41.40	25.91	PolyUnsat Ester
FO3h015	1.19	0.06	First Esterification
FO3h016	11.73	12.23	First Esterification
FO3h017	43.38	19.30	Clathration
FO3h018	6.07	2.78	Clath Raffinate
FO3h019	9.77	0.72	First Esterification
FO3h020	58.93	23.41	Mol Dist
FO3h021	10.62	5.18	MSC Pollock Oil
FO3h022	43.91	21.52	Separator
FO3h023	54.05	28.18	PolyUnsat Ester
FO3h024	0.00	0.00	First Esterification
FO3h025	26.97	12.82	First Esterification





Solo+Model_Exporter Workspace Browser

File Edit View Analyze Help FigBrowser New Version!

Current Folder: D:\PNA Data\300MHZ\OrgTech Fish Oils

Analysis Tools

Topics (double click to open)

- FAVORITES
 - DataSet Editor
 - Getting Started
 - PCA - Principal Component Analysis
- DECOMPOSITION
 - Batch Maturity
 - MCR - Multivariate Curve Resolution
 - MPCA - Multiway PCA
 - PARAFAC - Parallel Factor Analysis
 - PCA - Principal Component Analysis
 - SMMA - Purity
- REGRESSION
 - CLS - Classical Least Squares
 - LWR - Locally Weighted Regression
 - MLR - Multiple Linear Regression
 - MLR DOE - Designed Experiment MLR
 - NPLS - Multiway Partial Least Squares
 - PCR - Principal Component Regression
 - PLS - Partial Least Squares
 - SVM - Support Vector Machine
- CLUSTERING
 - Cluster Analysis
- CLASSIFICATION
 - KNN - K-Nearest Neighbor
 - PLSDA - Partial Least Squares Discriminant Analysis
 - SIMCA - Soft Independent Modeling of/by Class Analogy
 - SVMDA - Support Vector Machine Discriminant Analysis
- TRANSFORM
- OTHER
- TOOLS

EIGENVECTOR RESEARCH INCORPORATED

Workspace

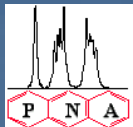
Current Workspace Variables

Name	Value	Byt
pls_modeljohnjohnnewhp_20130918t13340623	<PLS model>	425

Model Cache

Cache: "general" DATE View (* = Not Available)

- Cache Settings and View
- Demo Data
- 18-Sep-2013
 - item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:34:06.23
 - item: EPA GC Content - Sample 24 Removed.xlsx [49,1] "EPA"
 - item: NMR_FTIR Scaled - Sample 24 Removed.xlsx [49,977]
 - item: PLS (sim) 7 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:33:53.44
 - item: PLS (sim) 7 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:32:07.57
 - item: EPA GC Content - Sample 24 Removed.xlsx [49,1] "EPA"
 - item: NMR_FTIR Scaled - Sample 24 Removed.xlsx [49,1799]
 - item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:31:24.19
 - item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:30:48.50
 - item: EPA GC Content - Sample 24 Removed.xlsx [51,1] "EPA"
 - item: NMR_FTIR Scaled - Sample 24 Removed.xlsx [51,1799]
 - item: PLS (sim) 8 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:30:37.87
 - item: PLS (sim) 8 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:29:11.79
 - item: EPA GC Content - Sample 24 Removed.xlsx [53,1] "EPA"
 - item: NMR_FTIR Scaled - Sample 24 Removed.xlsx [53,1799]
 - item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:29:01.56
 - item: PLS (sim) 1 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:28:59.52
 - item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:23:02.05
 - item: EPA GC Content - Sample 24 Removed.xlsx [49,1] "EPA"



PROCESS NMR ASSOCIATES

Analysis - PLS (No Model)

File Edit Preprocess Analysis Tools Help FigBrowser

Analysis Flowchart

1. Load X data

2. Load Y data

Cache: "general" DATE View (* = Not Available)

Cache Settings and View

Demo Data

18-Sep-2013

item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:34:06.23

item: EPA GC Content - Sample 24 Removed.xlsx [49,1] "EPA"

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item: PLS (sim) 6 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:23:02.05

item: EPA GC Content - Sample 24 Removed.xlsx [49,1] "EPA"

item: NMR_FTIR Scaled - Sample 24 Removed.xlsx [49,1799]

item: PLS (sim) 1 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:23:00.05

item: PLS (sim) 5 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:21:58.84

item: EPA GC Content - Sample 24 Removed.xlsx [52,1] "EPA"

item: NMR_FTIR Scaled - Sample 24 Removed.xlsx [52,1799]

item: PLS (sim) 1 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 13:21:56.70

item: PLS (sim) 5 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 12:42:23.58

item: EPA GC Content.xlsx [49,1] "EPA"

item: aaa-1H-300MHz_IntelligentIntegrals.xlsx [49,11]

item: PLS (sim) 5 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 12:41:43.44

item: EPA GC Content.xlsx [53,1] "EPA"

item: aaa-1H-300MHz_IntelligentIntegrals.xlsx [53,11]

item: PLS (sim) 4 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 12:41:31.64

item: PLS (sim) 1 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 12:41:29.85

item: PLS (sim) 5 LVs [X: Mean Center] [Y: Mean Center] 2013-09-18 12:40:14.06

item: EPA GC Content.xlsx [50,1] "EPA"

item: aaa-1H-300MHz_IntelligentIntegrals.xlsx [50,11]

Click to import calibration X-block data

Number LVs: Auto Select

Percent Variance Captured by Model (* = suggested)

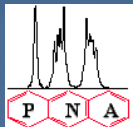
	X-Block LV	X-Block Cumulative	Y-Block LV	y-Block Cumulative
1				

Import

Import from file type:

- Excel File (XLS,XLSX,CSV,TXT)
- Experiment File (EXP,CSV,XLS,TXT)
- Text from Clipboard (CSV,TXT,XML)
- XML file (XML)
- AdventACT MTF File (MTF)
- AIT ASF File (ASF, AIF, BKH)
- AIT PIONIR File (PDF)
- Analytical Spectral Devices (ASD) Indico (V6 and V7)
- Grams Thermo Galactic File (SPC, DHB)
- Horiba JY Raman File (NGS, NGC)
- Horiba JY Aqualog File (DAT)
- JCAMP (DX,JDX)
- Omnics SPA File (SPA)
- Stellarnet ABS File (ABS)

OK Cancel



PROCESS NMR ASSOCIATES

Analysis - PLS 6 LVs - NMR_FTIR Scaled - Sample 24 Removed.xlsx, EPA GC Content - Sample 24 Removed.xlsx

File Edit Preprocess Analysis Tools Help FigBrowser

Cluster Model Calibration Test / Validation

View: SSQ Table iPLS Variable Selection

Number LVs: 6 Auto Select

Percent Variance Captured by Model (* = suggested)

	X-Block LV	X-Block Cumulative	Y-Block LV	Y-Block Cumulative	RMSECV EPA
1	87.67	87.67	91.49	91.49	6.0809
2	8.12	95.80	0.63	92.11	6.0253
3	3.86	99.66	0.99	93.10	5.8972
4	0.09	99.75	5.85	98.95	2.8037
5	0.06	99.81	0.56	99.51	1.9861
6	0.04	99.85	0.15	99.66	1.6253
7	0.01	99.87	0.14	99.80	1.5385
8	0.03	99.90	0.03	99.82	1.5085
9	0.02	99.92	0.03	99.85	1.4865
10	0.01	99.94	0.02	99.87	1.5294
11	0.02	99.95	0.02	99.90	1.6728
12	0.01	99.96	0.02	99.92	1.6936
13	0.01	99.97	0.02	99.94	1.688
14	0.00	99.97	0.03	99.97	1.7064
15	0.00	99.97	0.01	99.97	1.7516
16	0.00	99.98	0.01	99.98	1.7466
17	0.00	99.98	0.01	99.99	1.7551
18	0.00	99.98	0.00	99.99	1.7646
19	0.00	99.99	0.00	100.00	1.7934
20	0.00	99.99	0.00	100.00	1.7912

Analysis Flowchart

1. Load X data
2. Load Y data
3. Choose Preprocessing
4. Choose Cross-Validation
5. Build Model
6. Choose Components
7. Review Scores
8. Review Loadings

Review Model

Use Model

9. Load Test Data
10. Apply Model

Cache: "general" DATE View (* = Not A

- Cache Settings and View
- Demo Data
- 18-Sep-2013
- item: PLS (sim) 6 LVs [X: Mean C
- item: EPA GC Content - Sample
- item: NMR_FTIR Scaled - Sample
- item: PLS (sim) 7 LVs [X: Mean C
- item: PLS (sim) 7 LVs [X: Mean C
- item: EPA GC Content - Sample
- item: NMR_FTIR Scaled - Sample
- item: PLS (sim) 6 LVs [X: Mean C

Plot Contr...

File Edit View Plot FigBrowser

Fig 1: Samples/Scores ...

X Scores on LV 1 (87.6...

Y Scores on LV 2 (8.12...

Scores on LV 3 (3.869...

Scores on LV 4 (0.099...

Scores on LV 5 (0.069...

Scores on LV 6 (0.04...

Residuals (0.15%)

Z: none

Color By...

Plot Plot Type...

Select Tool

Q con Q con Ref.

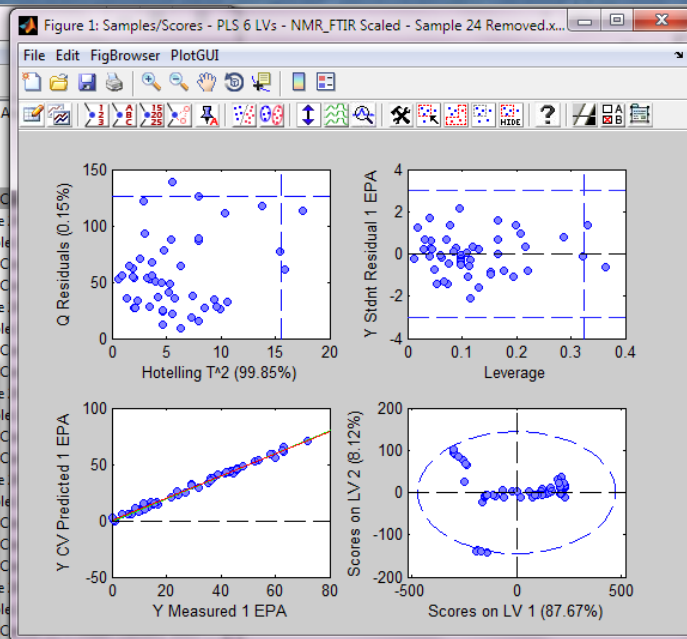
T con T con Ref.

data info

☒ Show Cal Data with Test

☐ Show Error Bars

☒ Conf. Limits: 95 %

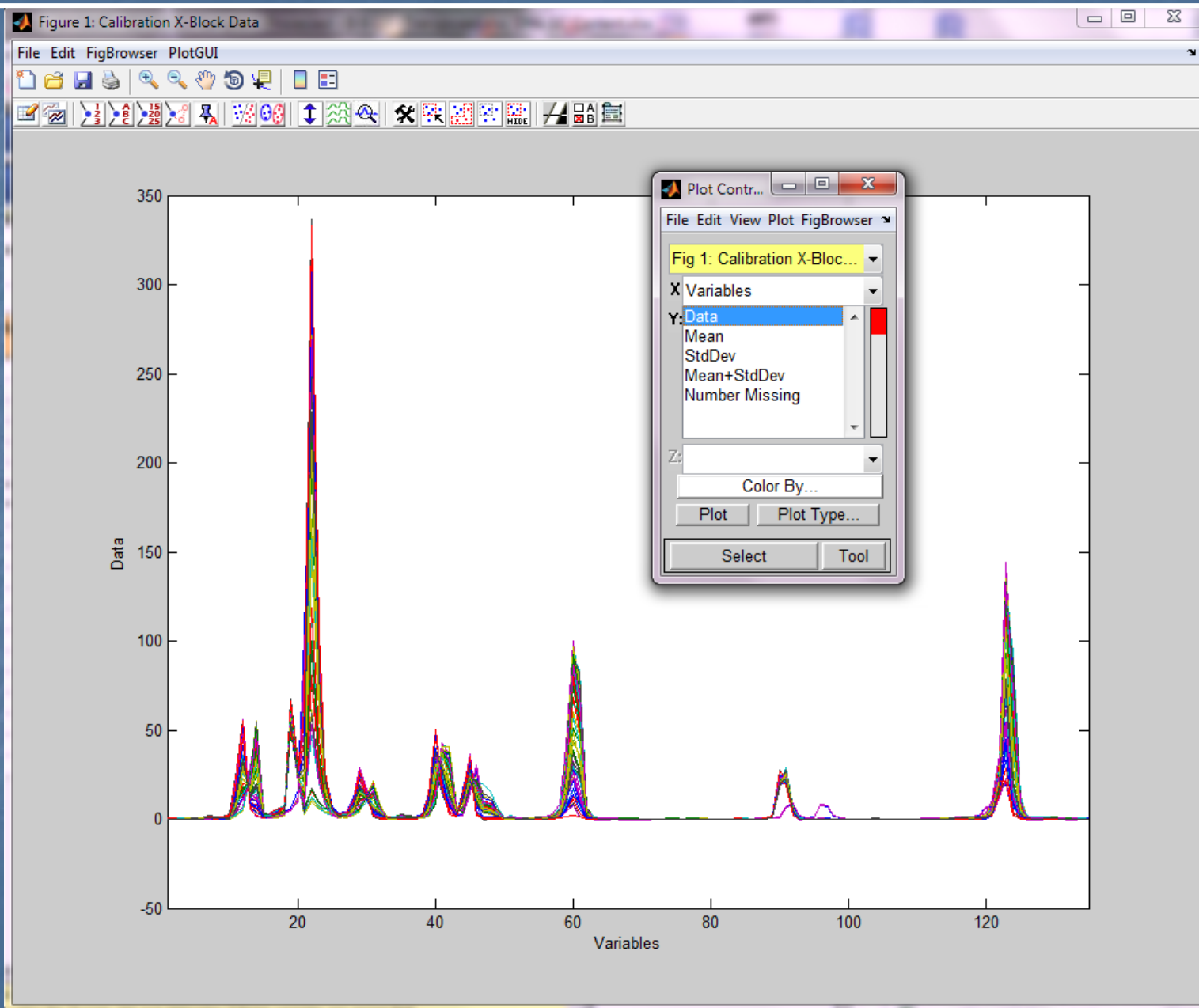


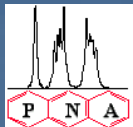
Center] [Y: Mean Center] 2013-
e 24 Removed.xlsx [52,1] "EPA"
le 24 Removed.xlsx [52,1799]
Center] [Y: Mean Center] 2013-
Center] [Y: Mean Center] 2013-
] "EPA"
Integrals.xlsx [49,11]
Center] [Y: Mean Center] 2013-
] "EPA"
Integrals.xlsx [53,11]
Center] [Y: Mean Center] 2013-
Center] [Y: Mean Center] 2013-
Center] [Y: Mean Center] 2013-
] "EPA"

item: aaa-1H-300MHz_IntelligentIntegrals.xlsx [50,11]
item: PLS (sim) 5 LVs [X: Mean Center] [Y: Mean Center] 2013-
item: EPA GC Content.xlsx [54,1] "EPA"



PROCESS NMR ASSOCIATES





PROCESS NMR ASSOCIATES

Acknowledgements

Paul Giammatteo – PNA

Tal Cohen – ASPECT AI and Modcon

Adam Dicaprio, Daniel Edwards – PNA

Mike Bernstein – MestreLabs (SMA Development)

For more information and applications visit www.process-nmr.com