

# Using JMP® Partial Least Squares to Model Chemometric (Near-Infrared Spectrometry) Data to Predict Percent Flavor on Coffee

Presented by:

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The J.M. Smucker Company



# Outline

- I. Introduction to Flavoring Coffee
- II. Gas-Chromatography vs. Near-Infrared (NIR)
- III. NIR Data in JMP
- IV. JMP Calibration Building
- V. Conclusions



# Introduction to Flavoring Coffee

- Liquid flavor is sprayed onto ground coffee in a large mix tank.
- Mixed for a set amount of time to ensure homogeneity.
- Test random samples throughout the packing line to verify proper distribution of the liquid flavor



# GC-MS

- Gas Chromatography – Mass Spectrometry
- Can use this analytical tool monitor key flavor markers in the headspace of the coffee.
- Have to create a multipoint calibration curve for each % flavor analysis to be conducted.
- Time Consuming - A single run can take up to 60 minutes to perform.
- Destructive to the sample.



# Near Infrared (NIR) Spectrometry

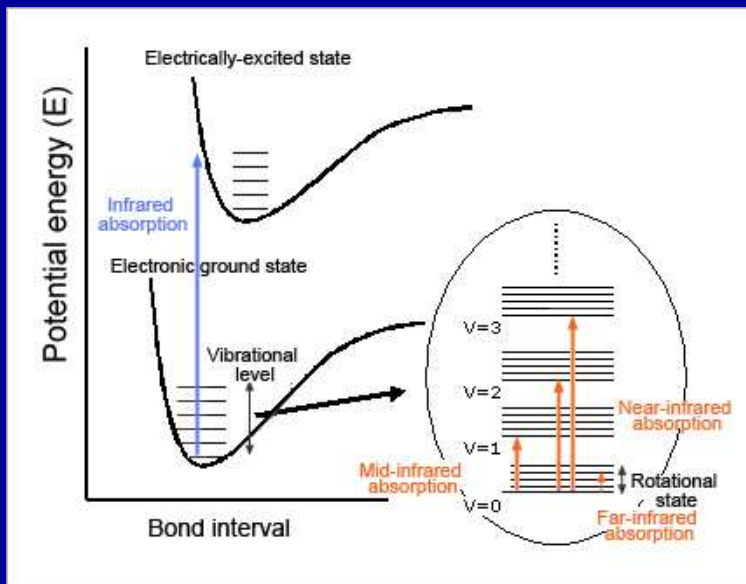
- Collect a spectra that fingerprints the flavored coffee sample.
- Quick – less than 2 minutes for a sample.
- Do not need to recreate a calibration curve each time % flavor analysis is required.
- Not destructive to the sample.





# What is NIR?

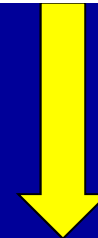
- The near-infrared (NIR) spectral region is usually defined as that portion of the spectrum with wavelengths in the range 700 to 2500nm.
- In this spectral region, overtone frequencies of molecular vibrations absorb light quite readily.
- Because the overtone absorption bands are typically wide and overlapping, spectroscopists cannot merely measure peak heights to perform quantitative analysis.
- Instead, multivariate regression analyses are utilized to correlate spectral features with concentrations or physical properties of interest.



# Work Flow



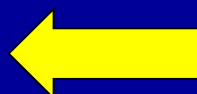
Export Data  
from NIR  
(.cal file)



“Clean Up”  
Data in JMP



Transpose  
Data in JMP



Create  
Calibration in  
JMP



# Data Collection

- A total of 41 spectra were collected from % flavor ranging from 2.5% to 5.5%.
- One spectra contains 1,050 data points.
- Performed 5 replicate NIR analysis on each calibration level.
  - 2.5%, 3.0%, 3.5%, 4.0%, 4.5%, 5.0% and 5.5%
  - Randomly collected 7 additional spectra from the 7 levels of calibration
- Want to be able to predict accurately within the 3% - 5% range.





# Export Data (.cal)

```
Percent Flavor.txt - Notepad
File Edit Format View Help

File ID:          Generated by ISIScan!
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Instrument Model: NIRSystems 6500
Serial No:        92400539      Samples:      41
Deleted:          0              Constituents: 1
No. Data Points: 1050          Moisture Basis Dry Matter
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# Import into JMP

Percent Flavor - JMP Conference - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Smucker's View Window Help

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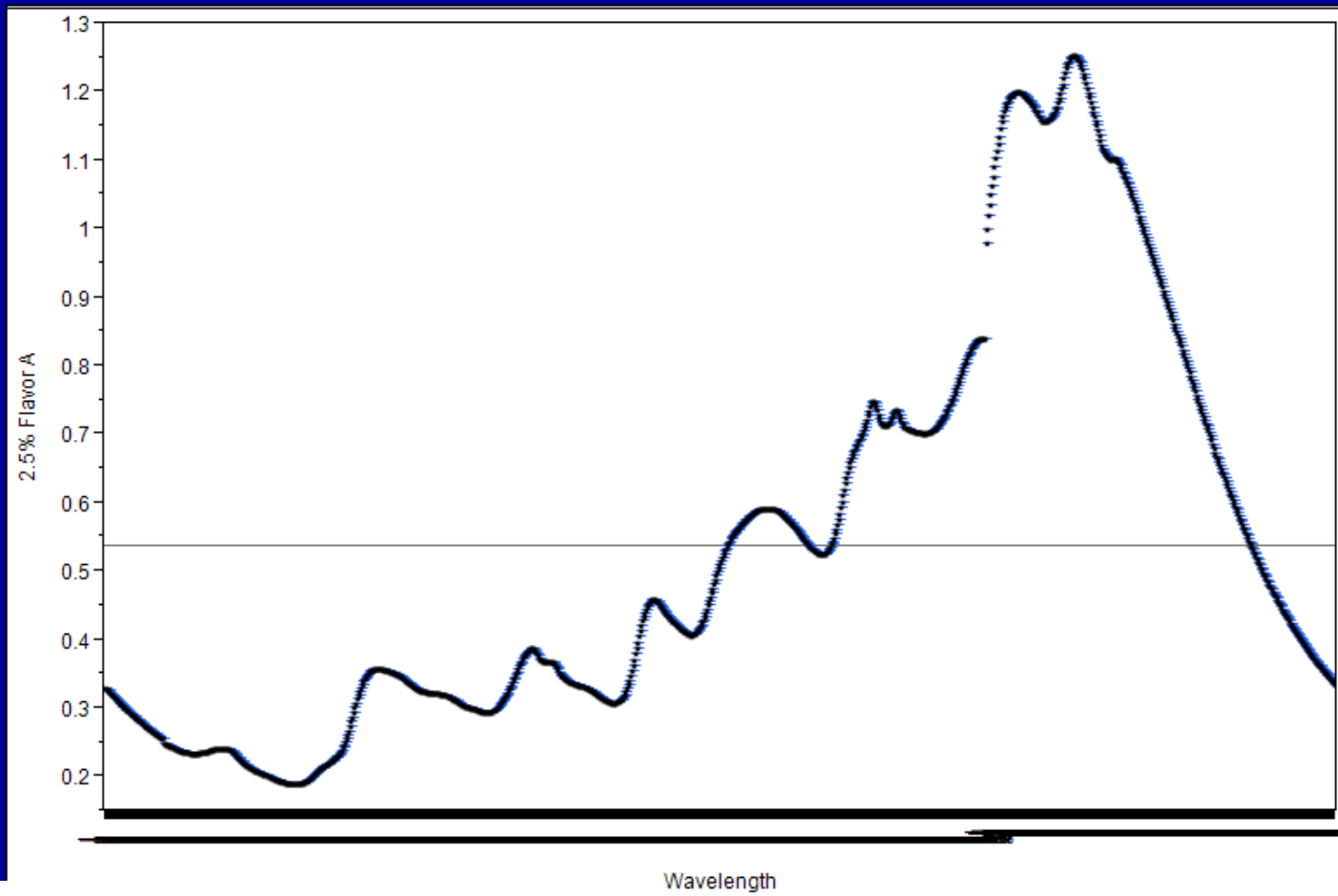
Columns (42/0)

- Wavelength
- 2.5% Flavor A
- 2.5% Flavor B
- 2.5% Flavor C
- 2.5% Flavor D
- 2.5% Flavor E
- 2.5% Flavor F
- 2.5% Flavor G
- 3.0% Flavor A
- 3.0% Flavor B
- 3.0% Flavor C
- 3.0% Flavor D
- 3.0% Flavor E
- 3.0% Flavor F
- 3.5% Flavor A
- 3.5% Flavor B
- 3.5% Flavor C

Rows

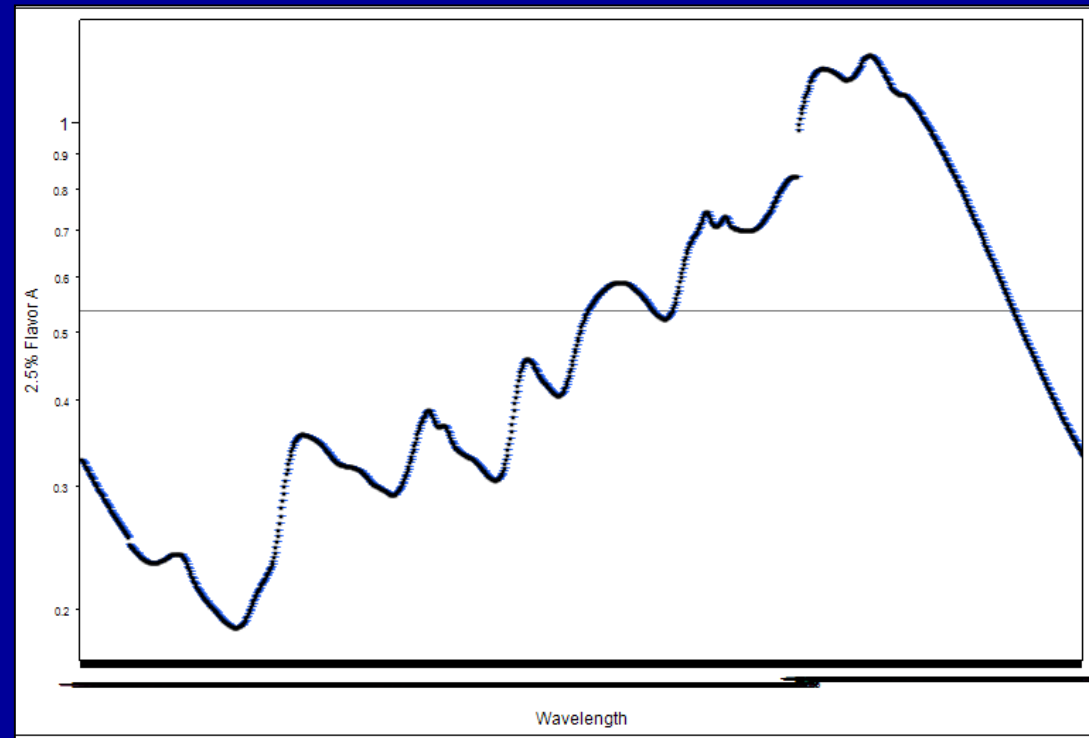
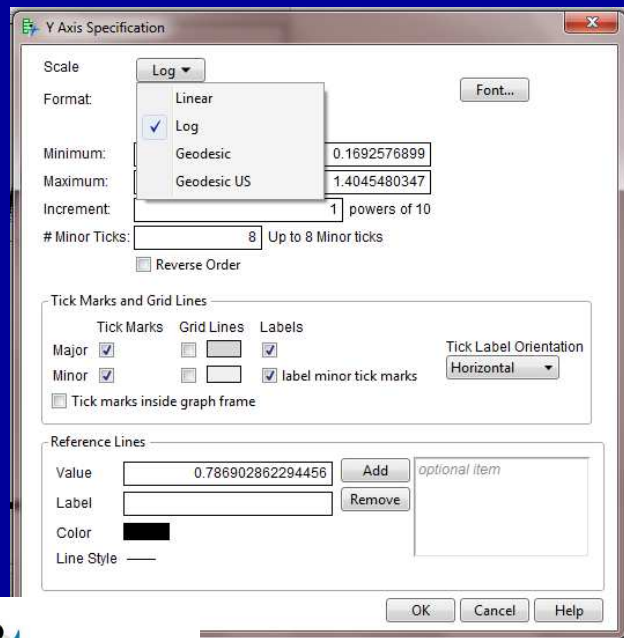
All rows 1,050  
Selected 0  
Excluded 0  
Hidden 0  
Labelled 0

# Check NIR Data Using Graph Builder



# Check NIR Data Using Graph Builder

Using the Y-Axis settings to change Y-Axis to log.  
To see proper NIR spectra





# Transpose the Data in JMP

The screenshot displays the JMP software interface with a data table titled "Percent Flavor - JMP". The table has columns for "Wavelength" and various "Flavor" percentages (2.5%, 3.0%, 3.5%). A "Transpose - JMP" dialog box is open, showing the "Interchange rows and columns" option. The "Select Columns" list includes "Wavelength" and all flavor columns. The "Transpose Columns" list contains "2.5% Flavor A", "2.5% Flavor B", "2.5% Flavor C", and "2.5% Flavor D". The "Label" field is set to "Wavelength" and the "By" field is set to "optional".

Wavelength	2.5% Flavor A	2.5% Flavor B	2.5% Flavor C	2.5% Flavor D	2.5% Flavor E	2.5% Flavor F	2.5% Flavor G	3.0% Flavor A	3.0% Flavor B	3.0% Flavor C	3.0% Flavor D	3.0% Flavor E	3.0% Flavor F	3.5% Flavor A	
1	0.98139	1.00079	1.0195	1.03689	1.05092	1.06364	1.07769	1.09135	1.10351	1.11354	1.12413	1.13510	1.14656	1.15675	
2	0.9877194	0.9941735	1.0012369	1.0096988	1.0084938	1.0253175	1.0126693	1.0201707	1.0156196	1.0271084	1.0430266	1.0299156	1.0375841	1.0328438	1.044598
3	1.0573626	1.0439048	1.0513976	1.0463502	1.0589802	1.0702996	1.056334	1.063972	1.058538	1.0720282	1.0843434	1.0701904	1.0779562	1.0727	1.0863519
4	1.097562	1.0838619	1.0913256	1.0866596	1.0999793	1.1092314	1.095696	1.103035	1.0983933	1.1117874	1.1195147	1.1057639	1.1129572	1.1081648	1.1217673
5	1.130355	1.1177459	1.1243238	1.1199985	1.1325494	1.1405299	1.1298981	1.1365237	1.1323438	1.1426642	1.1511265	1.1401927	1.1481324	1.1430852	1.152277
6	1.1619735	1.1483802	1.1573608	1.1517544	1.1621643	1.1715055	1.1559798	1.1648445	1.1596165	1.1726749	1.1789448	1.1632335	1.1718595	1.1669443	1.1816554
7	1.1847301	1.1694696	1.1779245	1.1730417	1.1878067	1.1886723	1.1737635	1.1820672	1.177253	1.191663	1.1923641	1.1776447	1.1862218	1.1813471	1.1957622
8	1.1962056	1.181293	1.1902645	1.185231	1.1997814	1.1990891	1.1839018	1.1927648	1.1876936	1.2021952	1.2016711	1.186563	1.1950891	1.1899922	1.2043595
9	1.2034078	1.1888182	1.1972497	1.192028	1.2061989	1.2048372	1.1908267	1.1991754	1.1939414	1.2078108	1.2063885	1.1923512	1.2004737	1.1953779	1.2091719
10	1.2078108	1.1930571	1.2011417	1.1961532	1.2102703	1.2080824	1.1926789	1.2010155	1.1959951	1.2105918	1.2076366	1.1923757	1.2008219	1.1955938	1.2105238
11	1.2069411	1.1922882	1.2006416	1.1951187	1.2102029	1.2060978	1.1918113	1.2004404	1.1946471	1.2097456	1.2090432	1.1927932	1.2009389	1.1959378	1.2090432

# The Transposed Data

Percent Flavor Transposed - JMP Conference - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Smucker's View Window Help

Percent Flavor Transp...  
 ▾ Principal Components  
 ▾ Actual vs. Predicted  
 ▾ Partial Least Squares

Columns (1051/0)  
 ▾ Percent Flavor  
 ▾ 400  
 ▾ 402  
 ▾ 404  
 ▾ 406  
 ▾ 408  
 ▾ 410  
 ▾ 412  
 ▾ 414  
 ▾ 416  
 ▾ 418  
 ▾ 420

Rows  
 All rows 41  
 Selected 0  
 Excluded 0  
 Hidden 0  
 Labelled 0

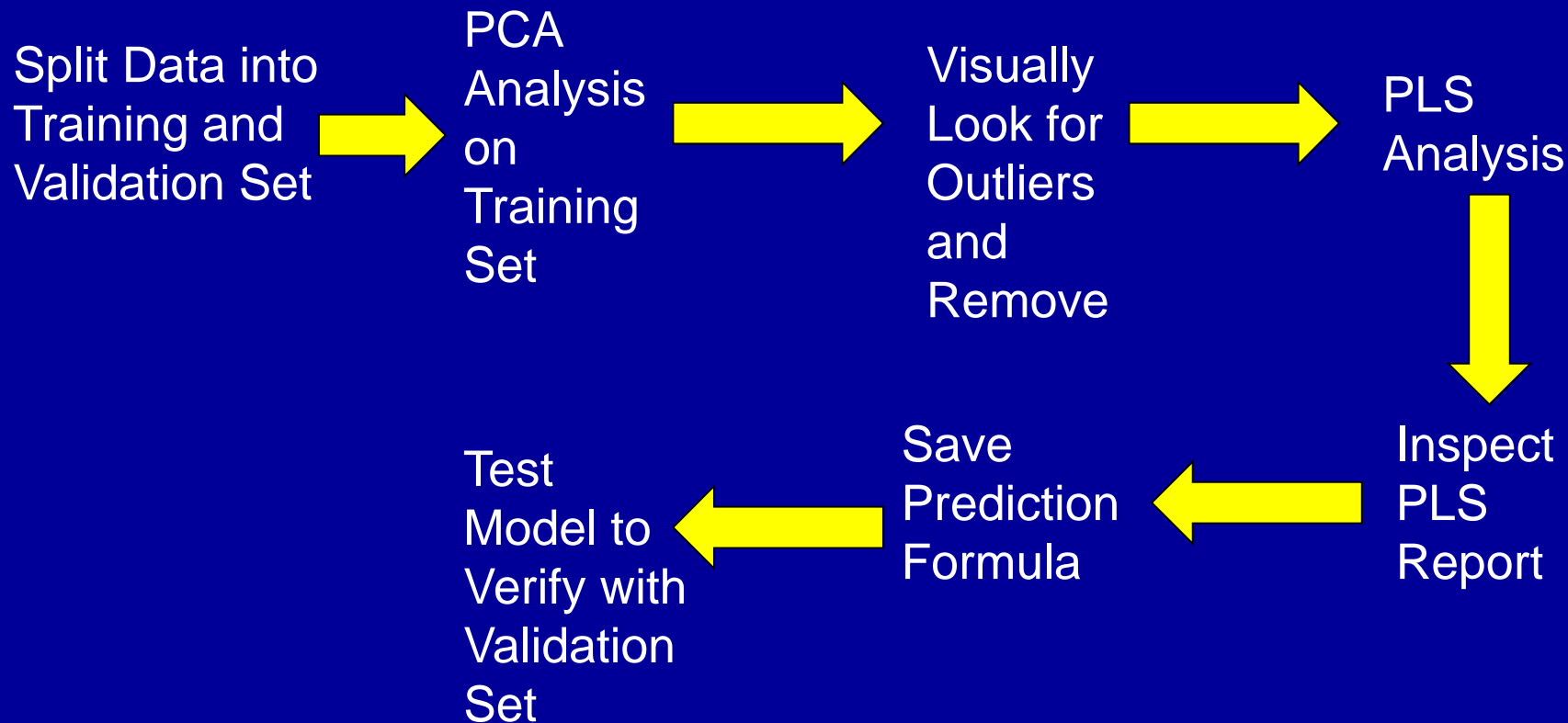
	Percent Flavor	400	402	404	406	408	410	412	414	416	418
1	2.5	0.9813938	1.0007919	1.019593	1.0368928	1.0509202	1.0636446	1.0776987	1.0913576	1.1035103	1.1135428
2	2.5	0.9842668	1.0027515	1.0201092	1.0372621	1.0531135	1.0683587	1.084043	1.0969658	1.1069919	1.1162021
3	2.5	0.9868069	1.005953	1.0246242	1.0419766	1.0564275	1.0698149	1.0842564	1.0977004	1.1094571	1.1196387
4	2.5	0.9762557	0.9953468	1.0138572	1.0309376	1.0448096	1.057497	1.0716701	1.0854098	1.0972898	1.1073644
5	2.5	0.9741375	0.9931396	1.0118532	1.0292882	1.0430632	1.0553675	1.0693994	1.0832607	1.0951856	1.1053472
6	2.5	0.973047	0.9917006	1.0101202	1.0272578	1.0405478	1.0525744	1.066649	1.0802858	1.0917902	1.102046
7	2.5	0.9783292	0.9972937	1.0159367	1.0333333	1.0471356	1.0594115	1.0733879	1.0873083	1.0993521	1.1091454
8	3	0.9920686	1.010829	1.0294138	1.0471839	1.06183	1.0748553	1.0889406	1.1023451	1.1140583	1.1242065
9	3	0.9931835	1.0122324	1.030789	1.0481575	1.0625222	1.0755997	1.0897958	1.1031731	1.1147739	1.1248944
10	3	0.9877194	1.0064559	1.0253175	1.0430266	1.0573626	1.0702996	1.0843434	1.097562	1.1092314	1.1195147
11	3	0.9750541	0.9941735	1.0126693	1.0299156	1.0439048	1.056334	1.0701904	1.0838619	1.095696	1.1057639
12	3	0.9820961	1.0012369	1.0201707	1.0375841	1.0513976	1.063972	1.0779562	1.0913256	1.103035	1.1129572
13	3	0.9780291	0.9969888	1.0156196	1.0328438	1.0463502	1.058538	1.0727	1.0866596	1.0983933	1.1081648
14	3.5	0.9893221	1.0084938	1.0271084	1.044598	1.0589802	1.0720282	1.0863519	1.0999793	1.1117874	1.1217673
15	3.5	1.021081	1.0386696	1.0560344	1.0725684	1.0862339	1.0986669	1.112427	1.125488	1.1367735	1.1463244
16	3.5	0.9921503	1.0108869	1.0293756	1.0468708	1.0612493	1.0743103	1.0886748	1.1023085	1.1139584	1.1237011
17	3.5	0.9810605	1.0003549	1.0192472	1.036625	1.050492	1.062917	1.0765345	1.0899477	1.1020734	1.1121554
18	3.5	0.9779345	0.9973192	1.0159171	1.0330797	1.0468979	1.0594349	1.0735109	1.0872569	1.0992117	1.1091394
19	4	0.9948151	1.0131482	1.0315982	1.049204	1.0633471	1.0760722	1.0902739	1.1038675	1.1156117	1.1254637
20	4	0.9917707	1.0108476	1.0294498	1.0467936	1.0609181	1.0737417	1.0878832	1.1014303	1.1133509	1.1235301
21	4	0.998576	1.017134	1.035308	1.0525937	1.066783	1.0798302	1.0943849	1.1080842	1.1197854	1.1297433
22	4	0.9887505	1.0072869	1.0254914	1.0428902	1.0572886	1.0700569	1.0838876	1.0973363	1.1093236	1.1192565
23	4	0.9799112	0.9988104	1.0173408	1.0347121	1.048558	1.0609128	1.0749121	1.0887041	1.1006423	1.1105404
24	4	0.9887742	1.0077679	1.0264139	1.0438069	1.0579097	1.0705922	1.084482	1.0979317	1.1099088	1.1199267
25	4.5	0.9899176	1.008806	1.0271853	1.0442063	1.0581596	1.0710049	1.0851965	1.098691	1.1105095	1.1206369
26	4.5	1.1122798	1.1274298	1.1414624	1.1546495	1.167057	1.1785451	1.1888965	1.1983147	1.2074349	1.2164179
27	4.5	0.9949094	1.0135708	1.0316792	1.0488031	1.0630057	1.075973	1.0902798	1.103784	1.1151903	1.1247408
28	4.5	0.9873857	1.0063657	1.0247977	1.0422082	1.0565391	1.069365	1.0833035	1.0967467	1.1087024	1.1187127
29	4.5	1.1381629	1.1528071	1.1674366	1.1811626	1.1918166	1.2014368	1.2128029	1.2238083	1.2330946	1.2405837
30	4.5	0.9925319	1.0114993	1.0300823	1.0476342	1.0618498	1.0743778	1.0881438	1.1016526	1.1138161	1.1241181
31	5	0.9933512	1.0119527	1.0304138	1.0478655	1.0620247	1.0749347	1.0894918	1.1027443	1.1149348	1.1259407

evaluations done

Show hidden icons



# Ready to Build A Calibration – JMP Work Flow



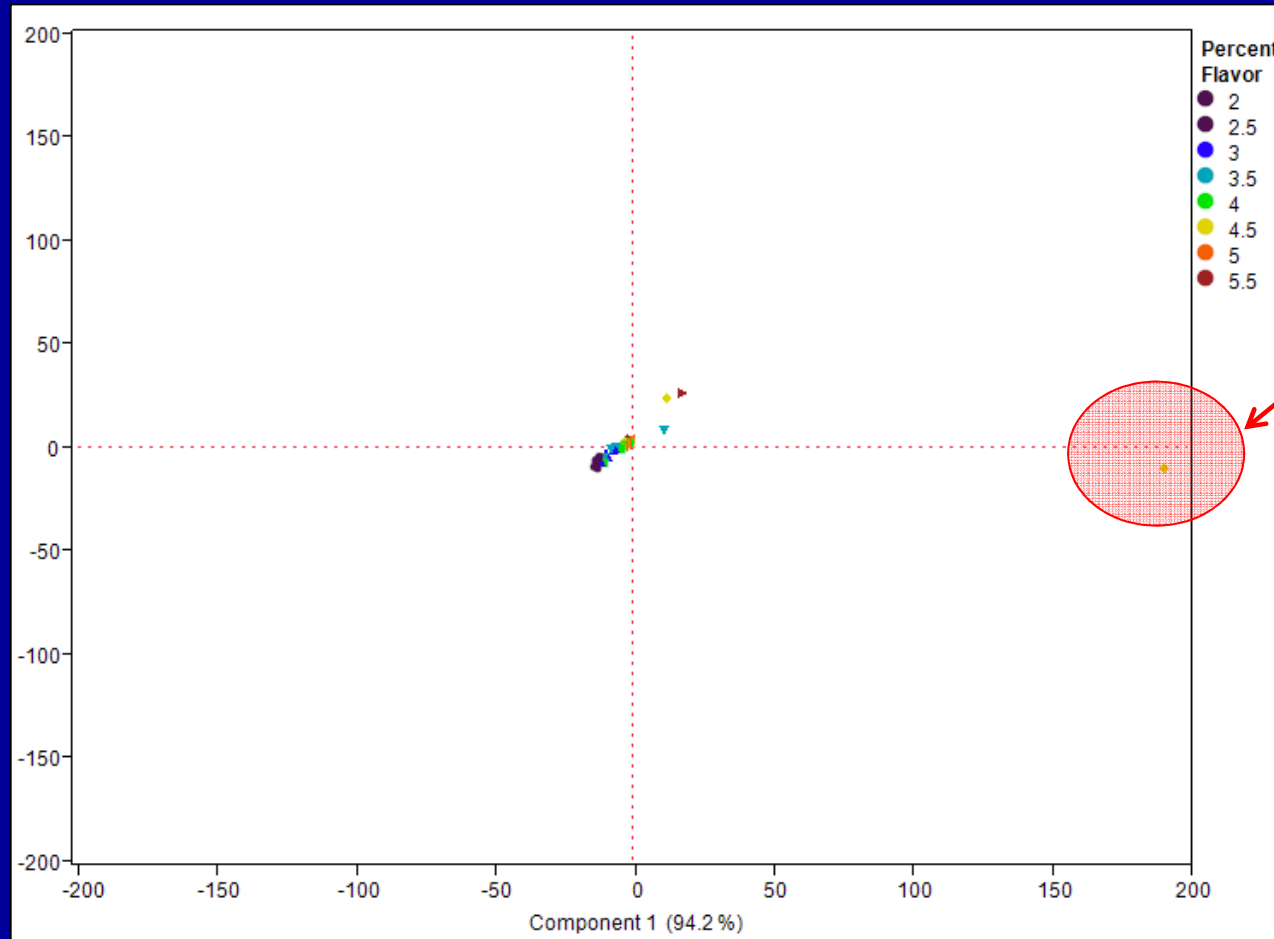
# Training vs. Validation Data

- Training Set
  - 27 spectra of the 41 collected randomly selected
  - 66% of the total data collected
- Training Set
  - 14 spectra of the 41 collected
  - 34% of the total data



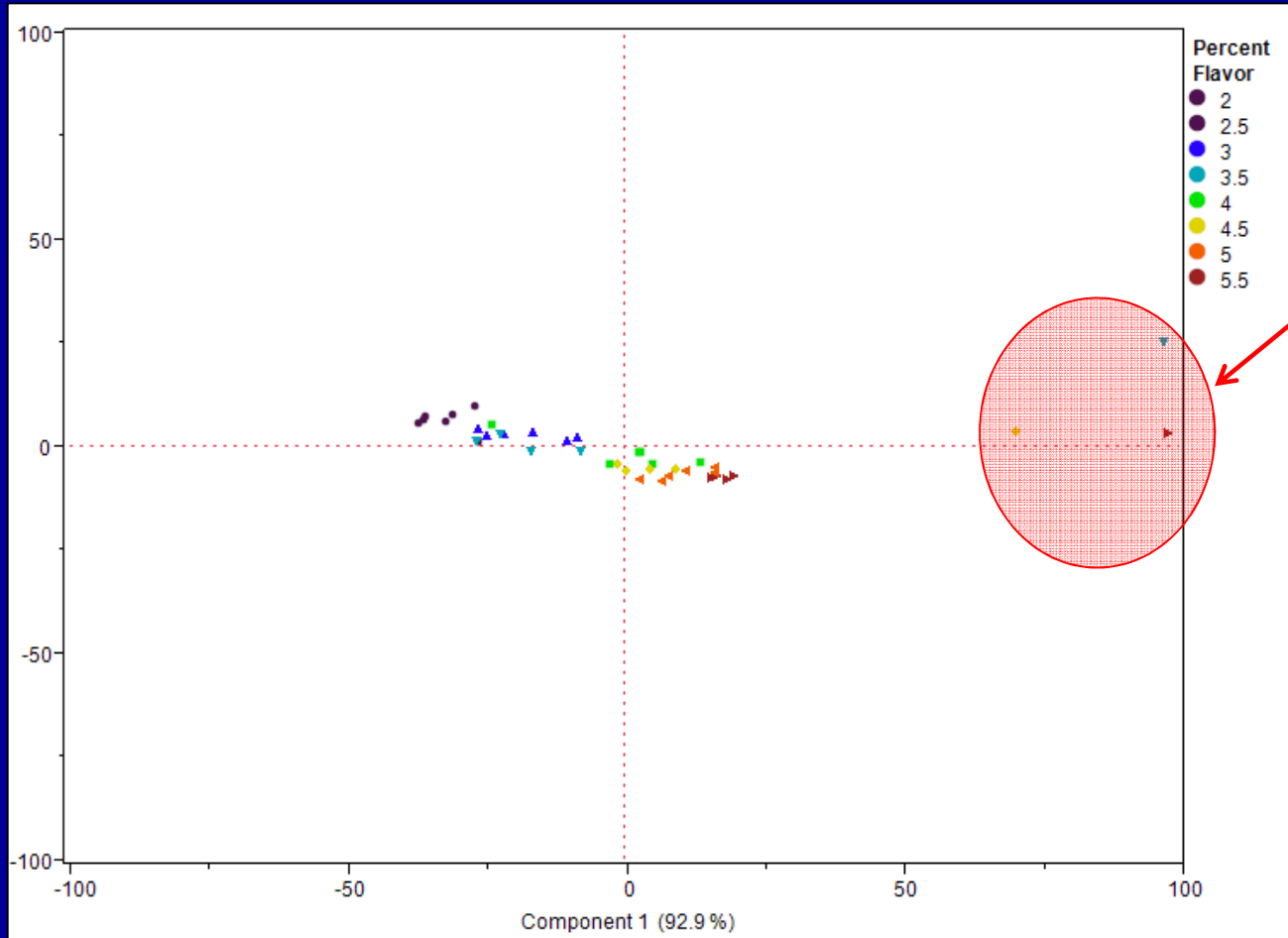


# PCA Analysis on Training Set



Outlier

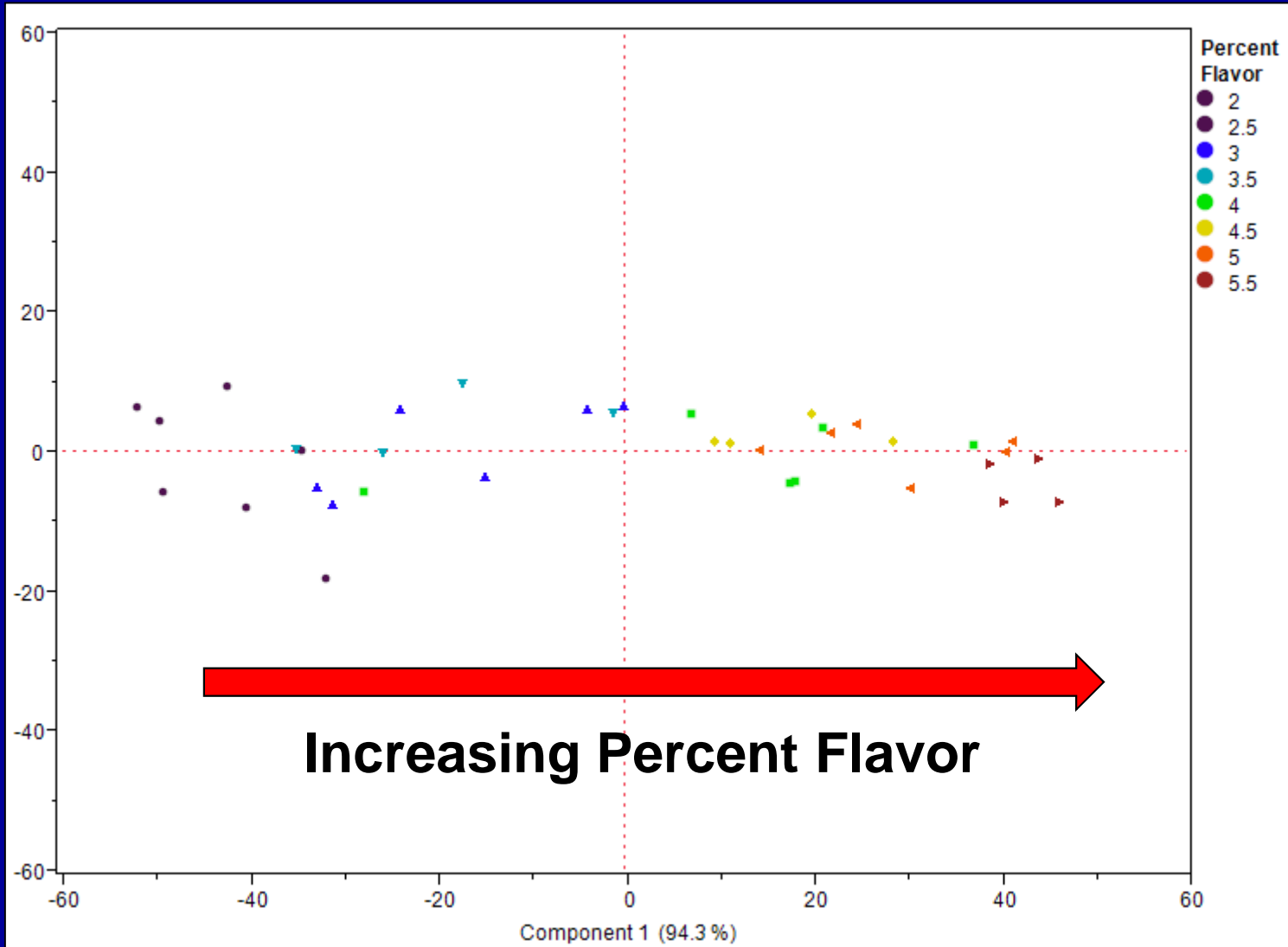
# PCA Analysis



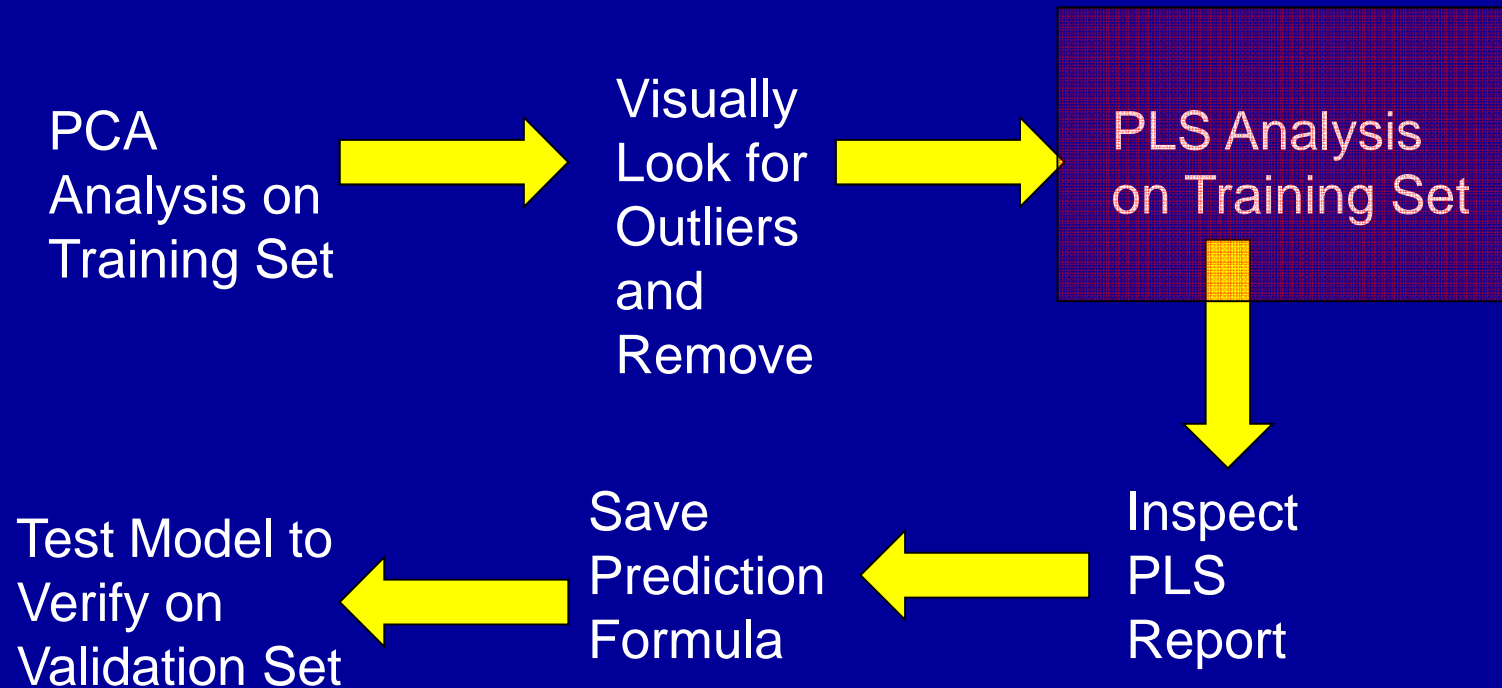
Outliers



# PCA Analysis



# Ready to Build A Calibration – JMP Work Flow



# Why a PLS Analysis?

- Partial least squares regression has been used in various disciplines such as chemistry, economics, medicine, psychology, and pharmaceutical science where predictive linear modeling, especially with a large number of predictors, is necessary.
- Especially in chemometrics, partial least squares regression has become a standard tool for modeling linear relations between multivariate measurements (de Jong, 1993).

de Jong, S (1993) SIMPLS: An Alternative Approach to Partial Least Squares Regression, *Chemometrics and Intelligent Laboratory Systems*, 18, 251-263



# PLS Analysis

Percent Flavor Transposed - JMP Conference - JMP

File Edit Tables Rows Cols DOE Analyze Graph Tools Smucker's View Window Help

Percent Flavor Transp...  
Partial Least Squares  
Principal Components  
Actual vs. Predicted

	Percent Flavor	400	Update 02	404	406	408	410	412	414	416	418
1	2.5	0.9813938	1.0007919	1.019593	1.0368928	1.0509202	1.0636446	1.0776987	1.0913576	1.1035103	1.1135428
2	2.5	0.9842668	1.0027515	1.0201092	1.0372621	1.0531135	1.0683587	1.084043	1.0969658	1.1069919	1.1162021
3	2.5	0.9868069	1.005953	1.0246242	1.0419766	1.0564275	1.0698149	1.0842564	1.0977004	1.1094571	1.1196387
4	2.5	0.9762557	0.9953468	1.0138572	1.0309376	1.0448096	1.057497	1.0716701	1.0854098	1.0972898	1.1073644
5	2.5	0.9741375	0.9931396	1.0118532	1.0292882	1.0430632	1.0553675	1.0693994	1.0832607	1.0951856	1.1053472
2578		1.0405478	1.0525744	1.066649	1.0802858	1.0917902	1.102046				
3333		1.0471356	1.0594115	1.0733879	1.0873083	1.0993521	1.1091454				
1839		1.06183	1.0748553	1.0889406	1.1023451	1.1140583	1.1242065				
1575		1.0625222	1.0755997	1.0897958	1.1031731	1.1147739	1.1248944				
0266		1.0573626	1.0702996	1.0843434	1.097562	1.1092314	1.1195147				
9156		1.0439048	1.056334	1.0701904	1.0838619	1.095696	1.1057639				
5841		1.0513976	1.063972	1.0779562	1.0913256	1.103035	1.1129572				
8438		1.0463502	1.058538	1.0727	1.0866596	1.0983933	1.1081648				
4598		1.0589802	1.0720282	1.0863519	1.0999793	1.1117874	1.1217673				
5684		1.0862339	1.0986669	1.112427	1.125488	1.1367735	1.1463244				
8708		1.0612493	1.0743103	1.0886748	1.1023085	1.1139584	1.1237011				
6625		1.050492	1.062917	1.0765345	1.0899477	1.1020734	1.1121554				
0797		1.0468979	1.0594349	1.0735109	1.0872569	1.0992117	1.1091394				
9204		1.0633471	1.0760722	1.0902739	1.1038675	1.1156117	1.1254637				
7936		1.0609181	1.0737417	1.0878832	1.1014303	1.1133509	1.1235301				
5937		1.066783	1.0798302	1.0943849	1.1080842	1.1197854	1.1297433				
8902		1.0572886	1.0700569	1.0838876	1.0973363	1.1093236	1.1192565				
7121		1.048558	1.0609128	1.0749121	1.0887041	1.1006423	1.1105404				
8069		1.0579097	1.0705922	1.084482	1.0979317	1.1099088	1.1199267				
2063		1.0581596	1.0710049	1.0851965	1.098691	1.1105095	1.1206369				
6495		1.167057	1.1785451	1.1888965	1.1983147	1.2074349	1.2164179				
		1.0630057	1.075973	1.0902798	1.103784	1.1151903	1.1247408				

Columns (1052/0)  
Percent Flavor  
400  
402  
404  
406  
408  
410  
412  
414  
416  
418

Rows  
All rows 41  
Selected 0  
Excluded 5  
Hidden 5  
Labelled 0

Partial Least Squares - JMP

Partial Least Squares

Select Columns  
Percent Flavor  
400  
402  
404  
406  
408  
410  
412  
414  
416  
418  
420  
422  
424  
426

Cast Selected Columns into Roles  
Y, Response: Percent Flavor (optional numeric)  
X, Factor: 400, 402, 404, 406 (optional)  
By: (optional)

Action  
OK  
Cancel  
Remove  
Recall  
Help

Centering  
 Scaling



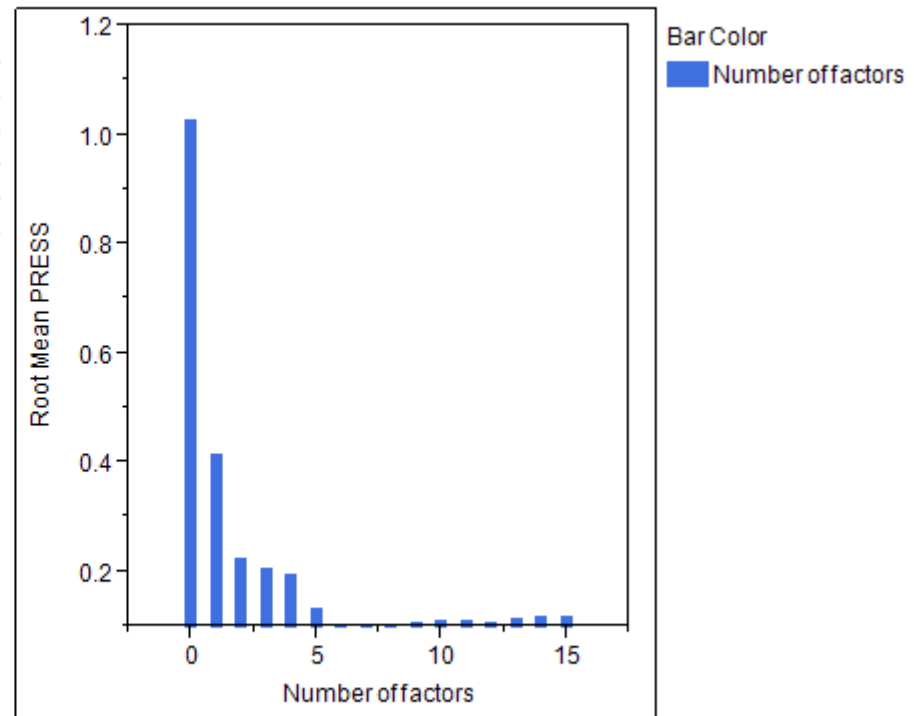
# PLS Analysis

## Model Comparison Summary

Method	Number of rows	Number of factors	Percent Variation Explained for Cumulative X	Percent Variation Explained for Cumulative Y	Number of VIP > 0.8
NIPALS	35	6	99.921109	99.509523	1050

## Cross Validation with Method=NIPALS

Number of factors	Root Mean PRESS	van der Voet T <sup>2</sup>	Prob > van der Voet T <sup>2</sup>
0	1.029412	20.860516	<.0001*
1	0.415187	12.223062	<.0001*
2	0.225024	11.449546	<.0001*
3	0.207357	11.406232	0.0010*
4	0.194286	11.097644	<.0001*
5	0.133627	5.486372	0.0110*
6	0.105026	0.325255	0.6030
7	0.101463	0.000000	1.0000
8	0.103153	0.116199	0.7380
9	0.108223	0.862401	0.3970
10	0.112024	1.277339	0.3010
11	0.109413	0.677987	0.4580
12	0.106051	0.167643	0.7300
13	0.116015	1.007926	0.3800
14	0.118630	1.265987	0.3160
15	0.117919	1.325740	0.3140

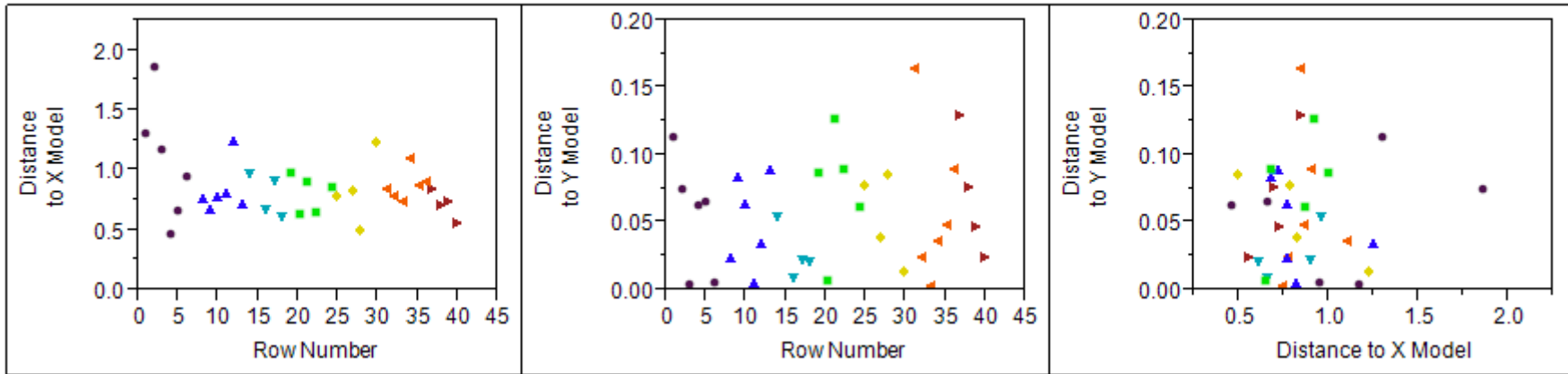


Note: The minimum root mean PRESS is 0.10146 and the minimizing number of factors is 7.



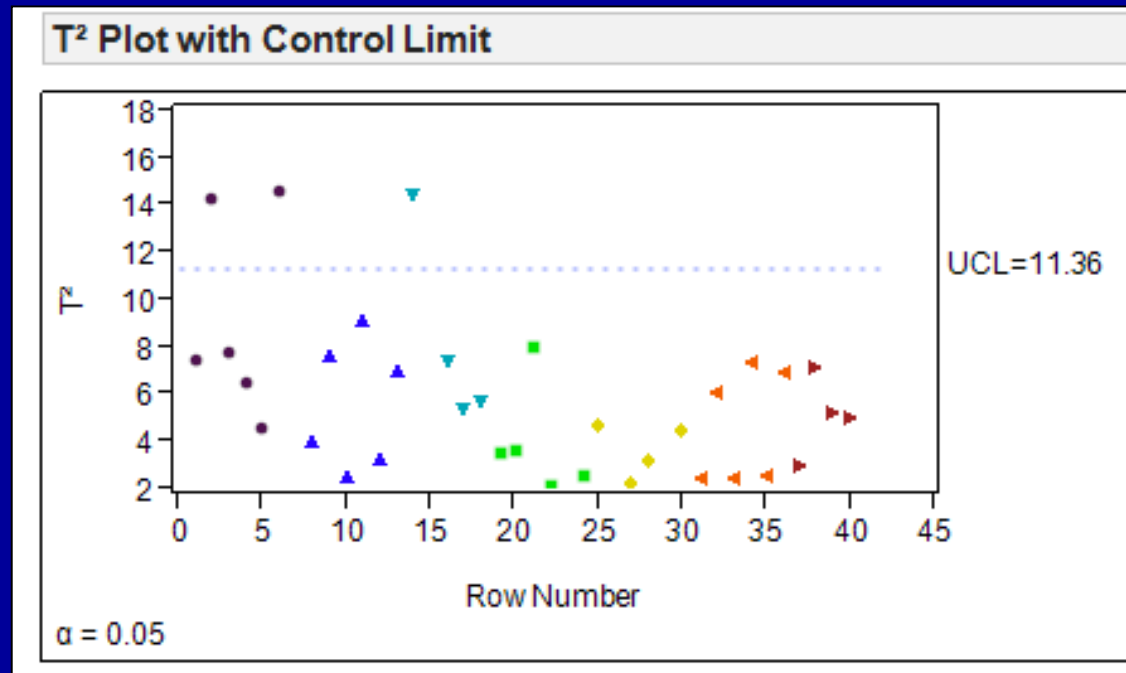
# Distance Plot Analysis

Distance Plots

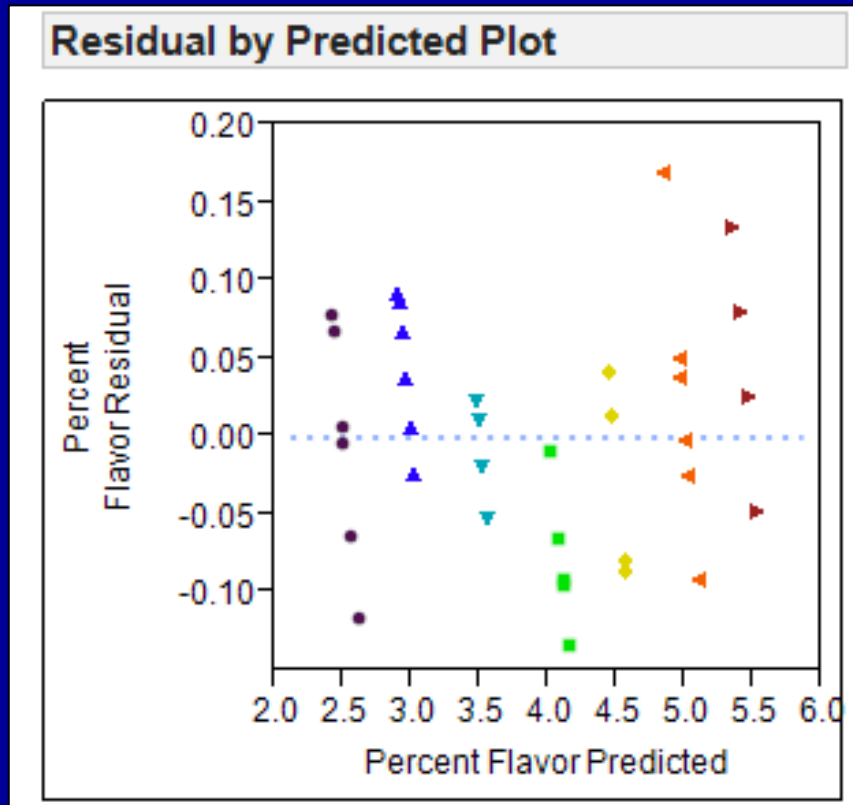




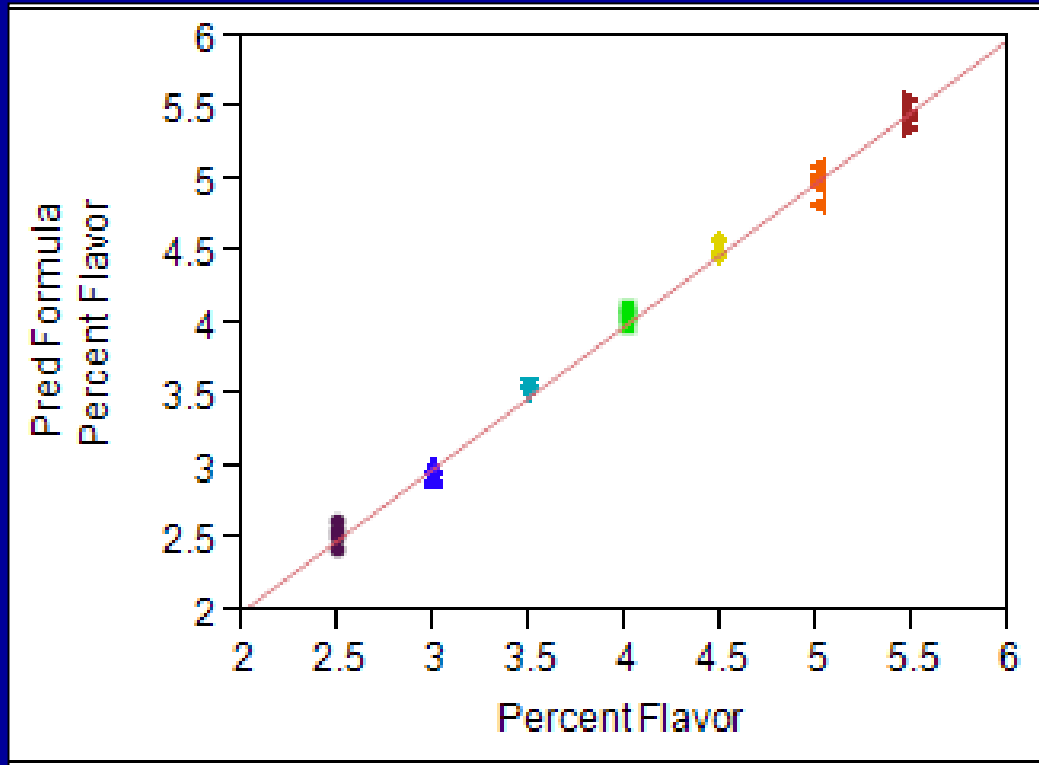
# T<sup>2</sup> Plot Analysis



# Residual Plot



# Actual vs. Predicted Plot



## Summary of Fit

RSquare	0.995095
RSquare Adj	0.994947
Root Mean Square Error	0.073214
Mean of Response	3.914286
Observations (or Sum Wqts)	35

## Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	35.888204	35.8882	6695.149
Error	33	0.176891	0.0054	Prob > F
C. Total	34	36.065094		<.0001*



# Predictive Formula

Pred Formula Percent Flavor - JMP

Table Columns

- Pred Formula P
- Percent Flavor
- 400
- 402
- 404
- 406
- 408
- 410
- 412

Functions (grouped)

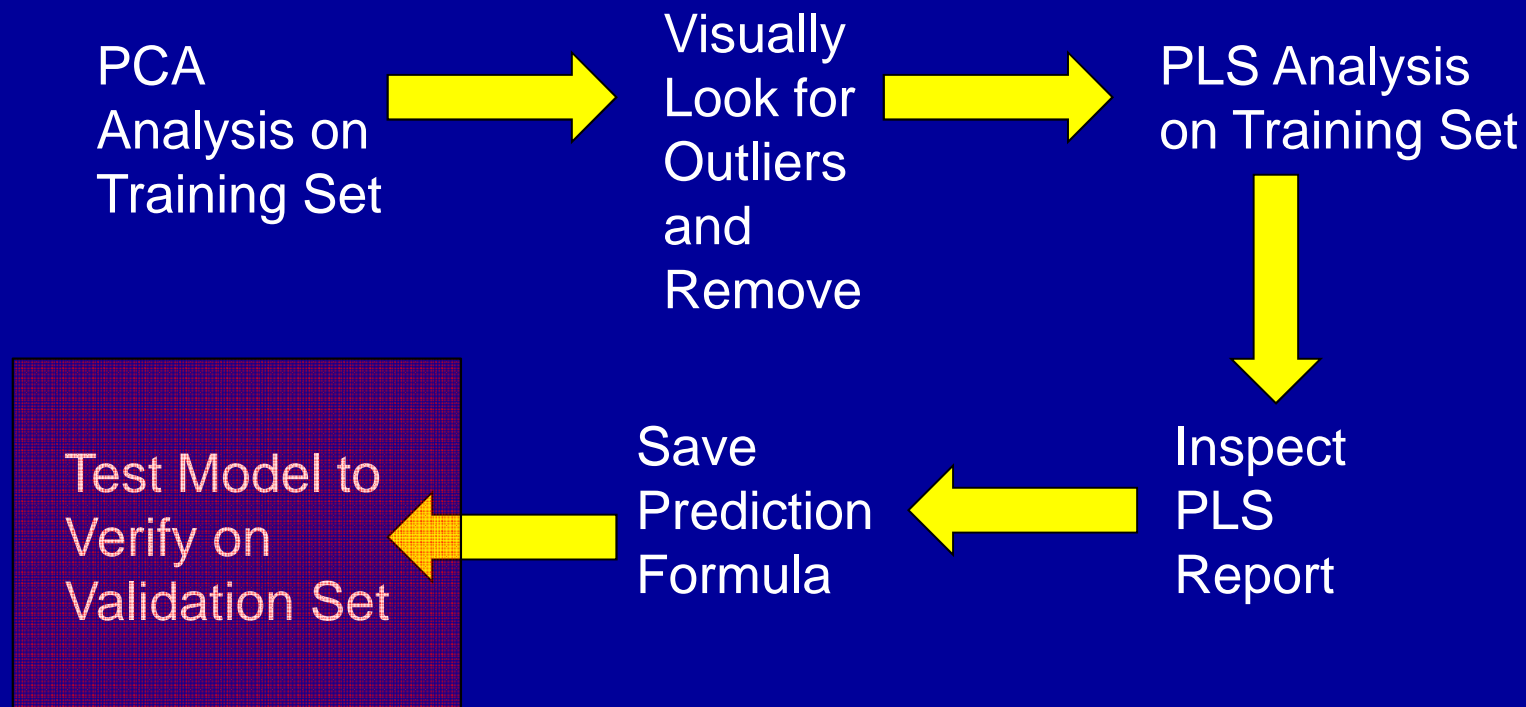
- Row
- Numeric
- Transcendental
- Trigonometric
- Character
- Comparison
- Conditional
- Probability
- Discrete Probability

OK  
Cancel  
Apply  
Clear  
Help

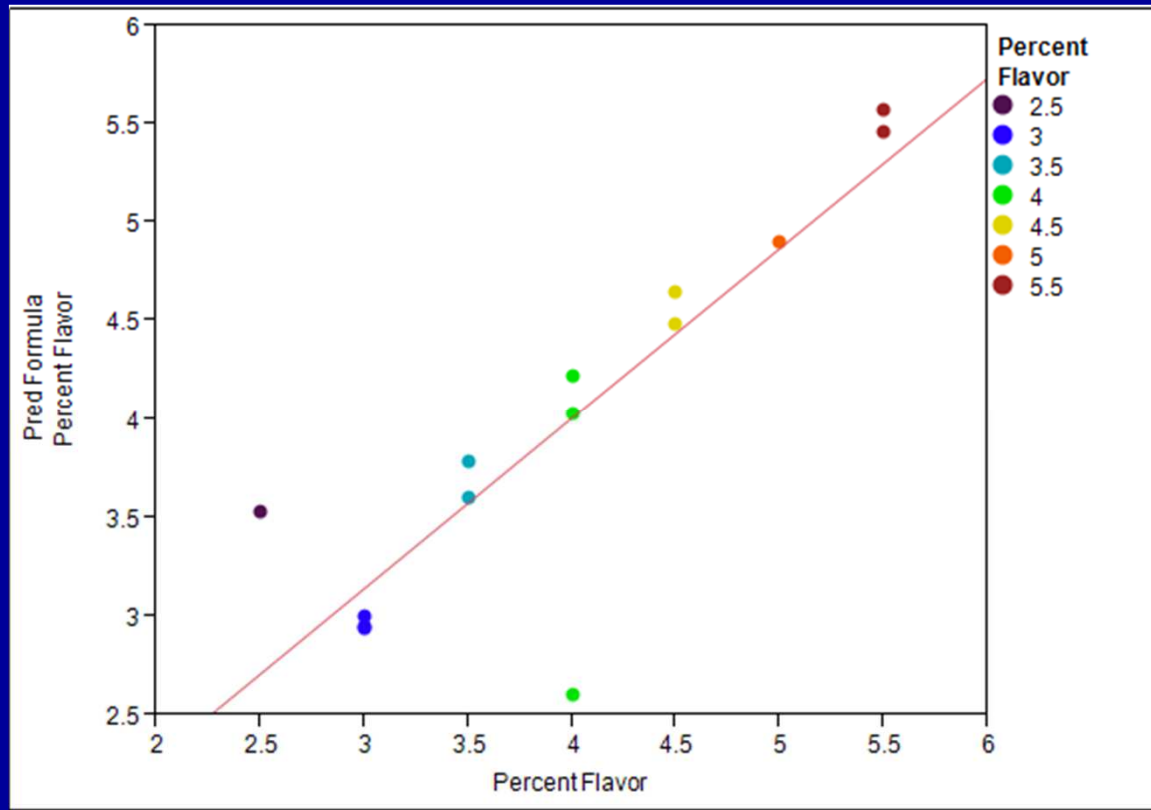
$-3.7348649248067 * 400$   
+  $-3.1958543753346 * 402$   
+  $-1.6179926352158 * 404$   
+  $-0.9773594425045 * 406$   
+  $-1.3386084552366 * 408$   
+  $-2.0970880138916 * 410$   
+  $-3.1612741236294 * 412$   
+  $-3.7555825706125 * 414$



# Ready to Build A Calibration – JMP Work Flow



# Validation Test



## Summary of Fit

RSquare	0.747404
RSquare Adj	0.726354
Root Mean Square Error	0.497297
Mean of Response	3.979467
Observations (or Sum Wqts)	14

## Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	8.780921	8.78092	35.5066
Error	12	2.967646	0.24730	Prob > F
C. Total	13	11.748567		<.0001*

## Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob> t
Intercept	0.5498443	0.590708	0.93	0.3703
Percent Flavor	0.86513	0.145187	5.96	<.0001*



# Conclusions

- Can build a calibration of % flavor from NIR data collected.
- JMP has the ability to handle complex analysis instrumentation data
- Must keep up and maintain calibration to ensure it keeps its accuracy and predicability.





**THANK YOU**

Thank you....

And any  
questions?

