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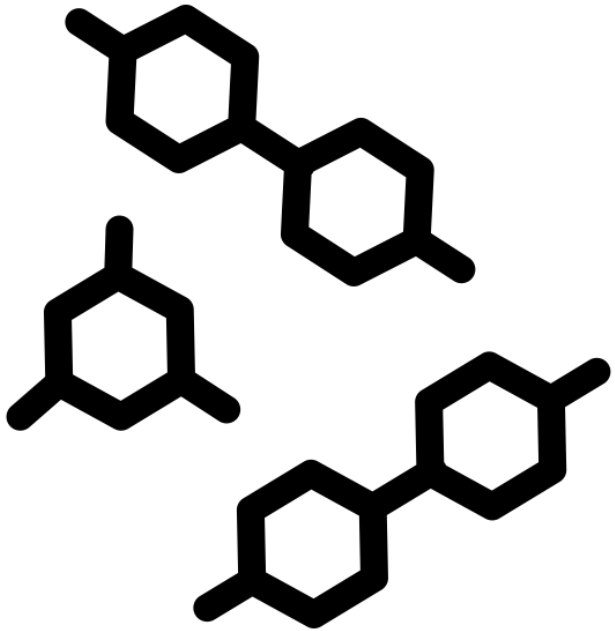
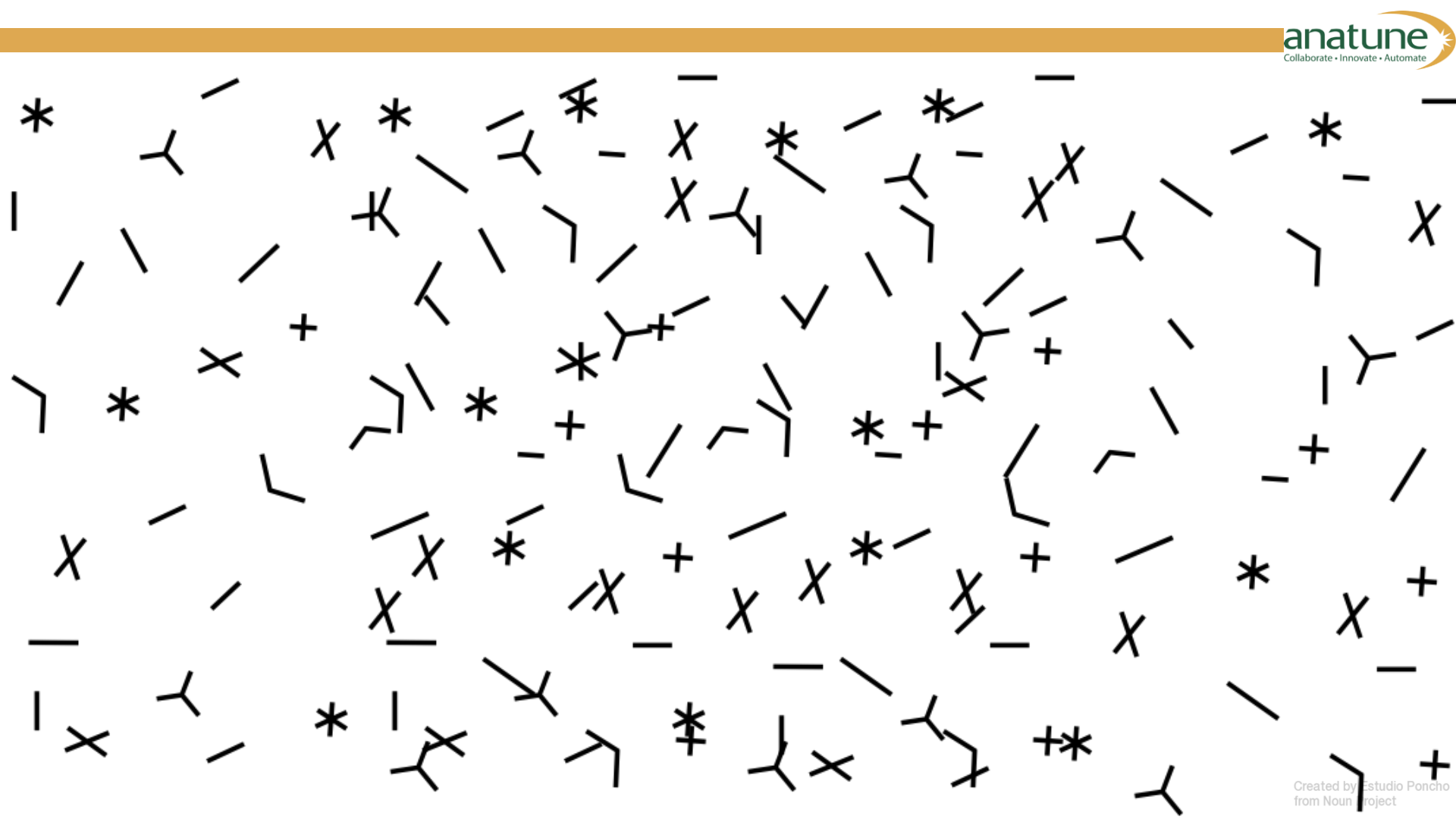
SIFTomics and data analytics:

The quickest way to unravel
the totality of your chemical space

Camilla Liscio, PhD
Senior Application Chemist

CHEMICAL SPACE

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from Noun Project

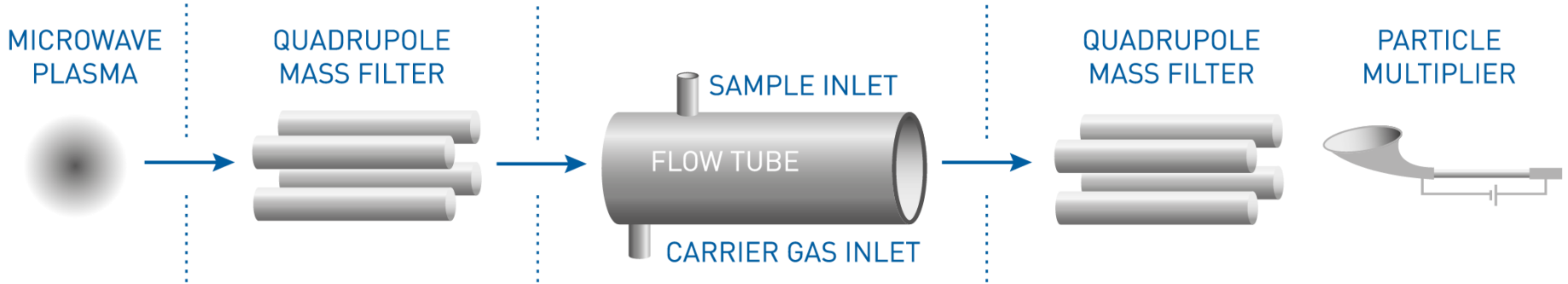
SUITABILITY SENSITIVITY SELECTIVITY SPEED

Selected Ion Flow Tube Mass Spectrometry (SIFT-MS)

Reagent Ion Selection

Analyte Ionization

Analyte Quantitation



Multiple reagent ions

Pure reagent ion delivery

Ultra-soft sample ionization

Mass spectrometer

SUITABILITY

Designed for both technical and non-technical personnel

SELECTIVITY

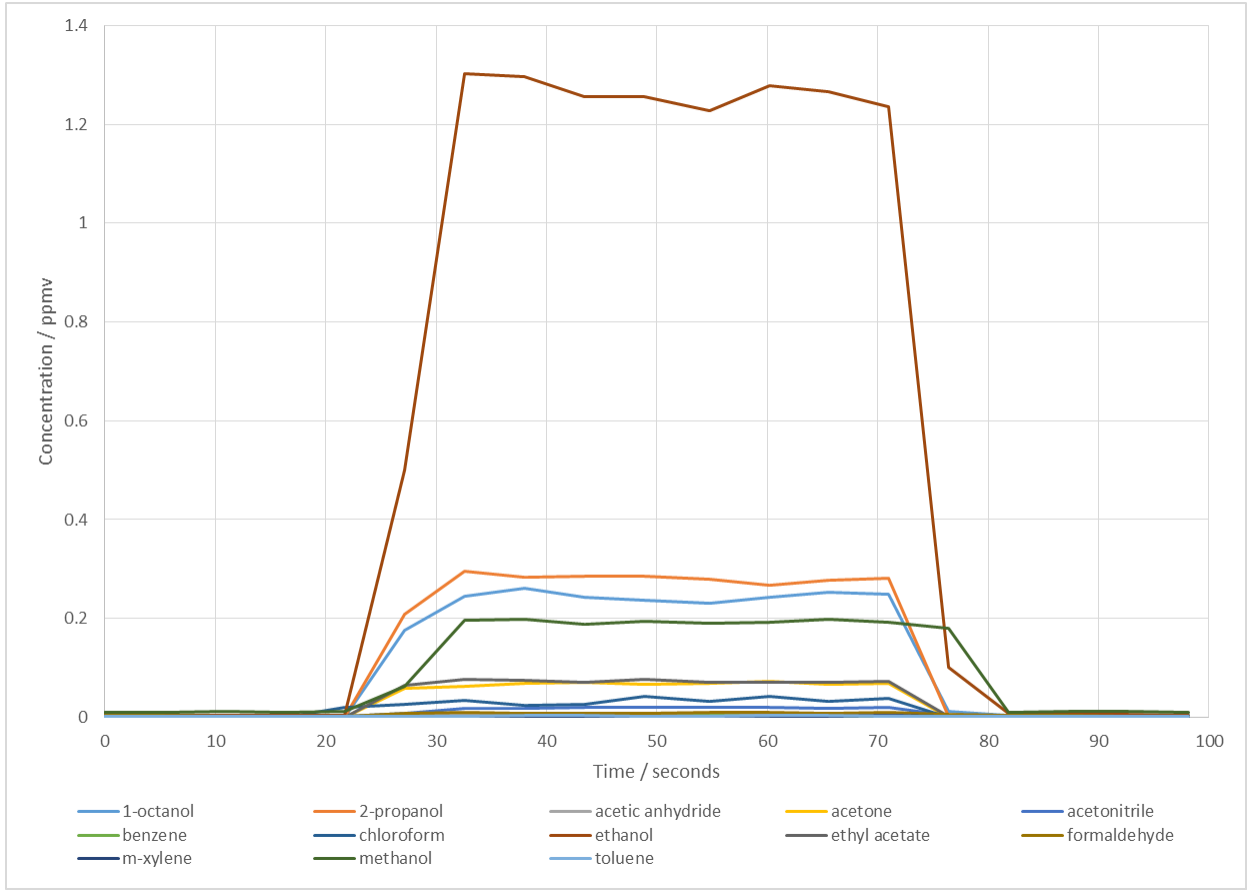
Analyzes chemically diverse species with high selectivity

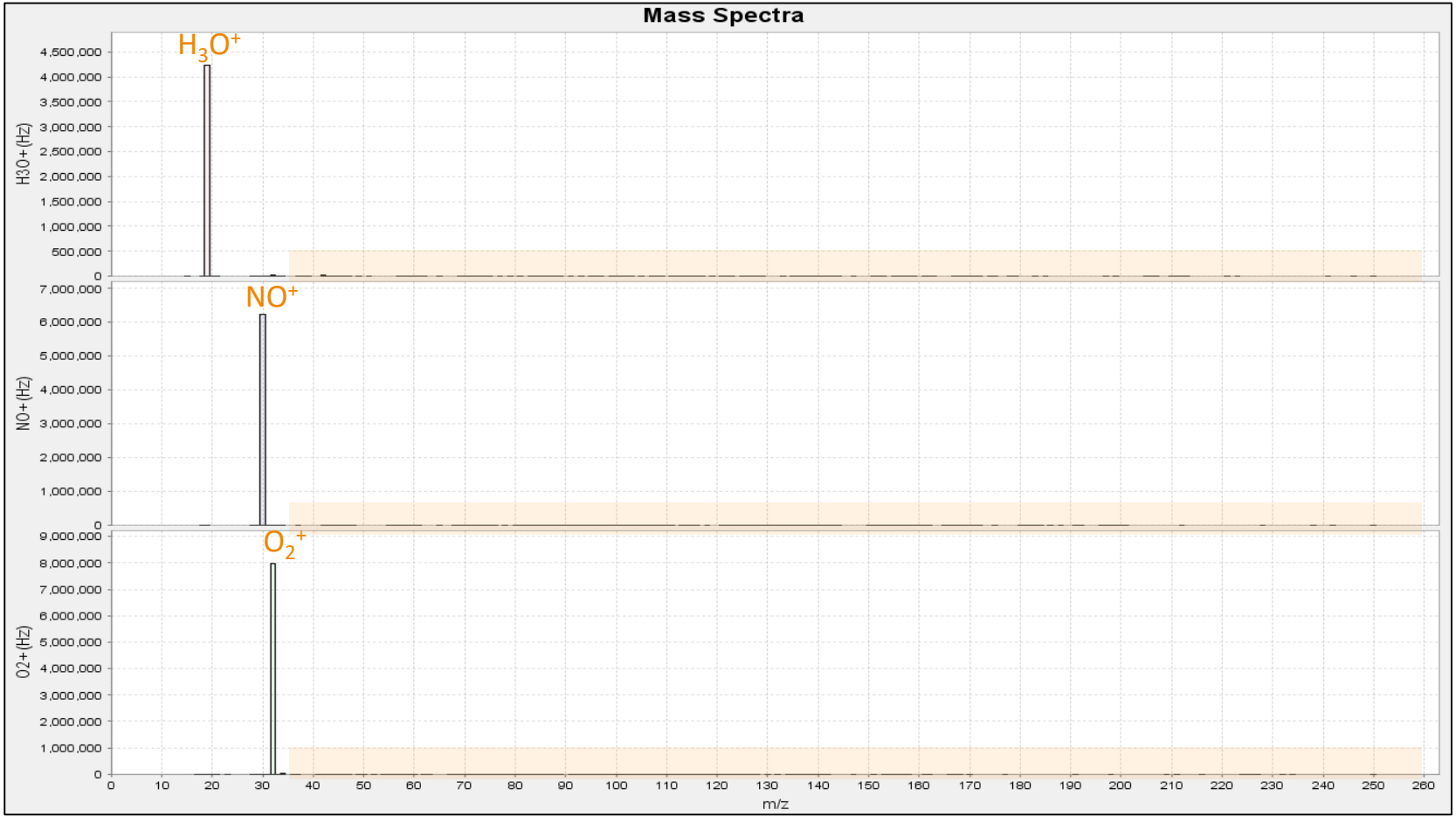
SENSITIVITY

Sensitive to pptv levels

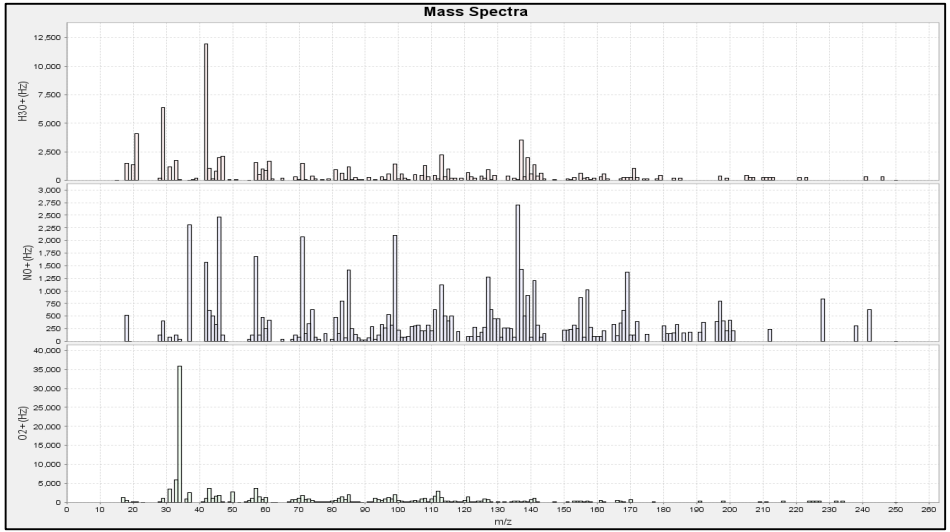
SPEED

Fast analysis and high throughput

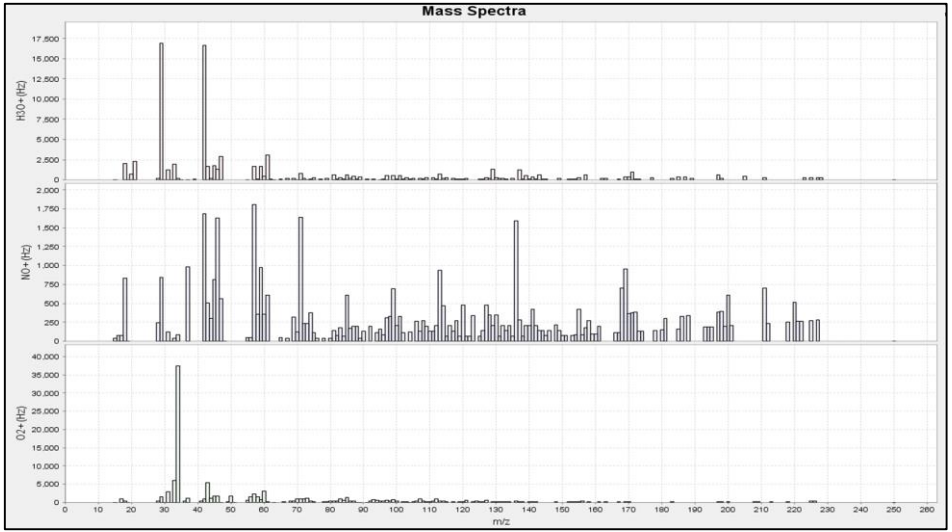

1.4
1.2
1
0.8
0.6
0.4
0.2
0
Concentration / ppmv
0
10
20
30
40
50
60
70
80
90
100
Time / seconds
1-octanol
2-propanol
acetic anhydride
acetone
acetonitrile
benzene
chloroform
ethanol
ethyl acetate
formaldehyde
m-xylene
methanol
toluene

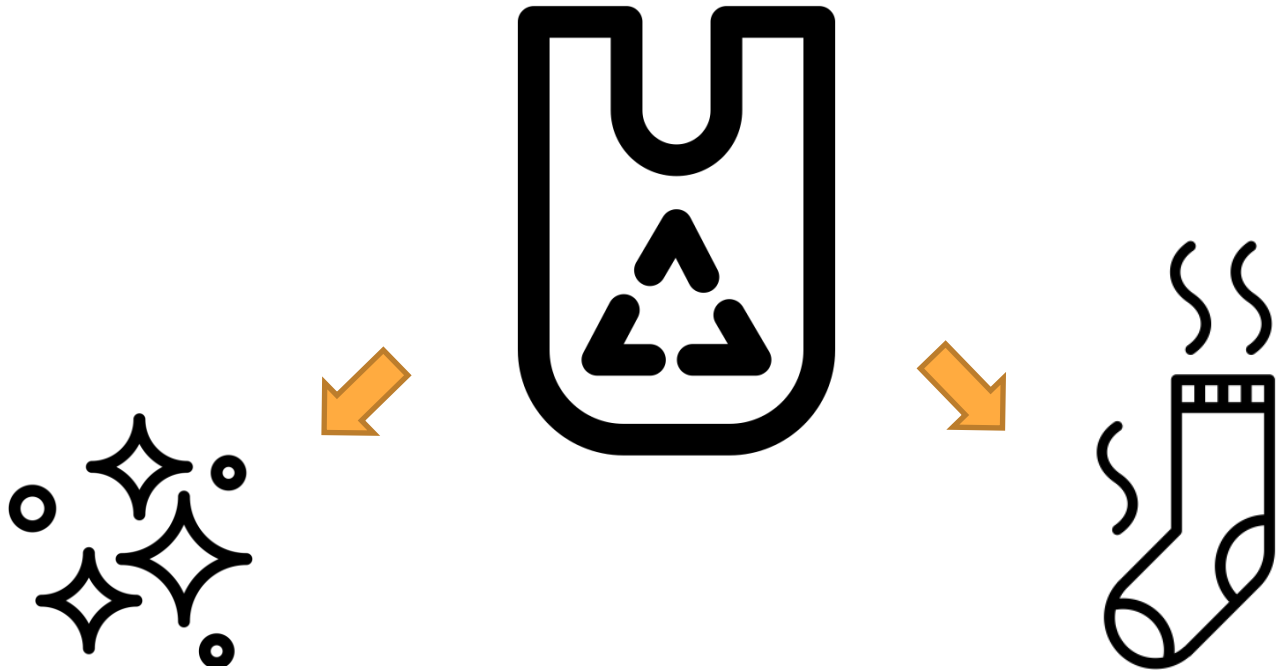

Mass Spectra
H_3O^+
H3O+ (Hz)
4,500,000
4,000,000
3,500,000
3,000,000
2,500,000
2,000,000
1,500,000
1,000,000
500,000
0
NO^+
NO+ (Hz)
7,000,000
6,000,000
5,000,000
4,000,000
3,000,000
2,000,000
1,000,000
0
O_2^+
O2+ (Hz)
9,000,000
8,000,000
7,000,000
6,000,000
5,000,000
4,000,000
3,000,000
2,000,000
1,000,000
0
0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260
m/z

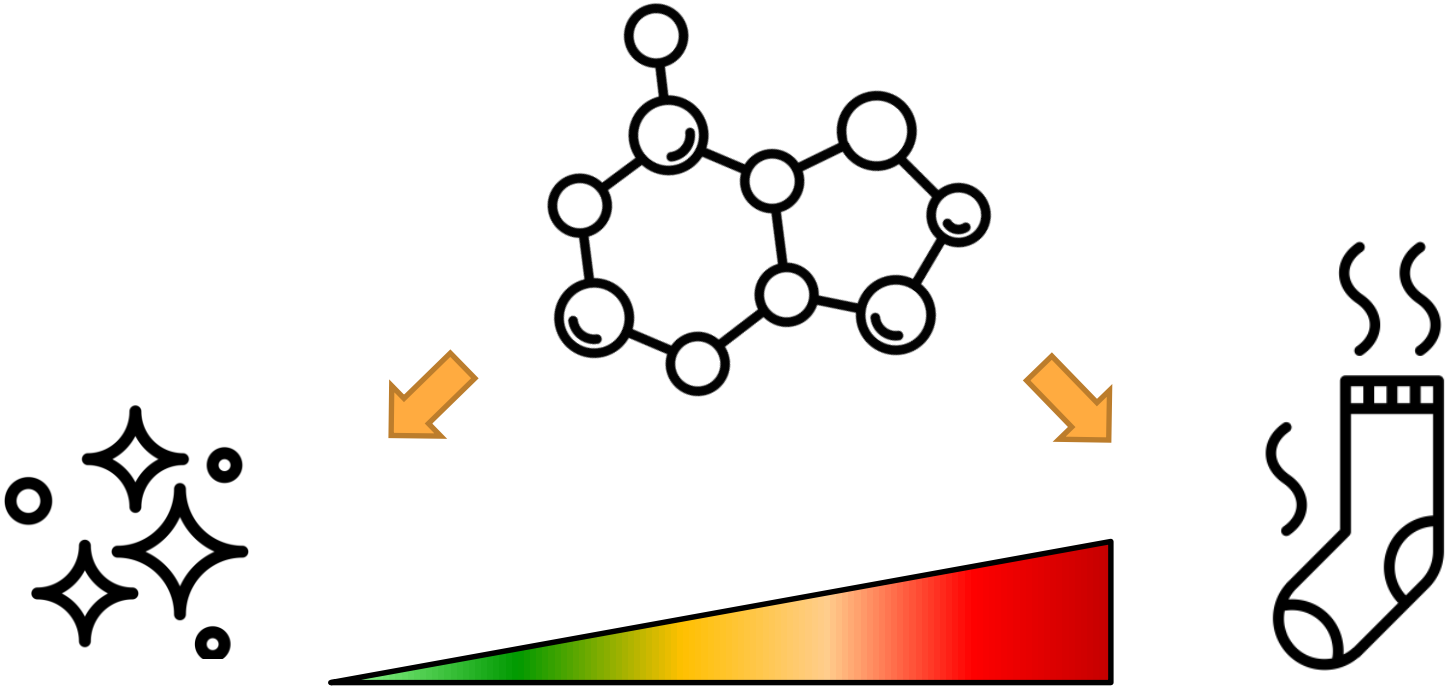
Sample A



Sample B



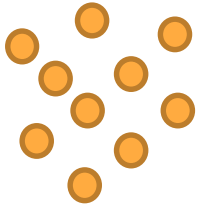




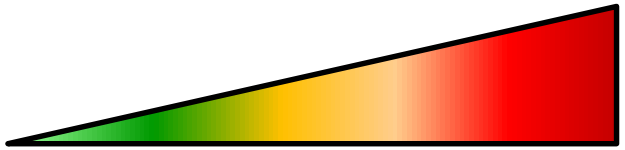
The Samples

22

n=10



Sensory Score



Sensory Score

Sample No. 5 C	Sample No. 10 Sample No. 9 Sample No. 11 Sample No. 8	Sample No. 6 Sample No. 7 Sample No. 16 Sample No. 18 Sample No. 12 Sample No. 4	Sample No. 19 Sample No. 21	Sample No. 3 Sample No. 14 Sample No. 15	Sample No. 1 Sample No. 2 D	Sample No. 20

The dataset

Reagent Ion Selection

MICROWAVE PLASMA

H_3O^+

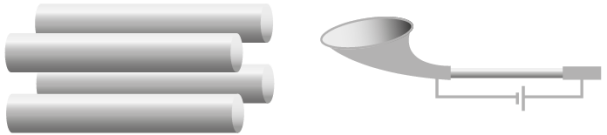
NO^+

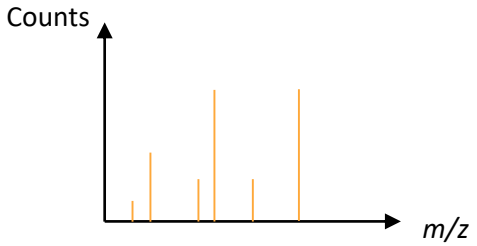
O_2^+

Analyte Quantitation

QUADRUPOLE MASS FILTER

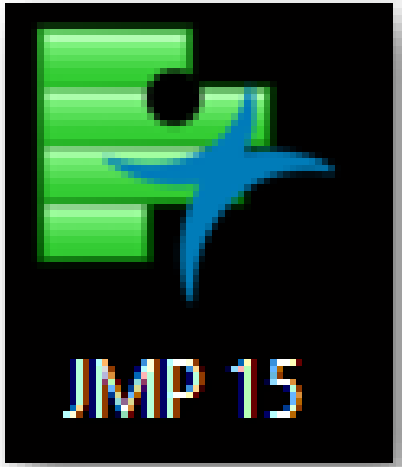
PARTICLE MULTIPLIER

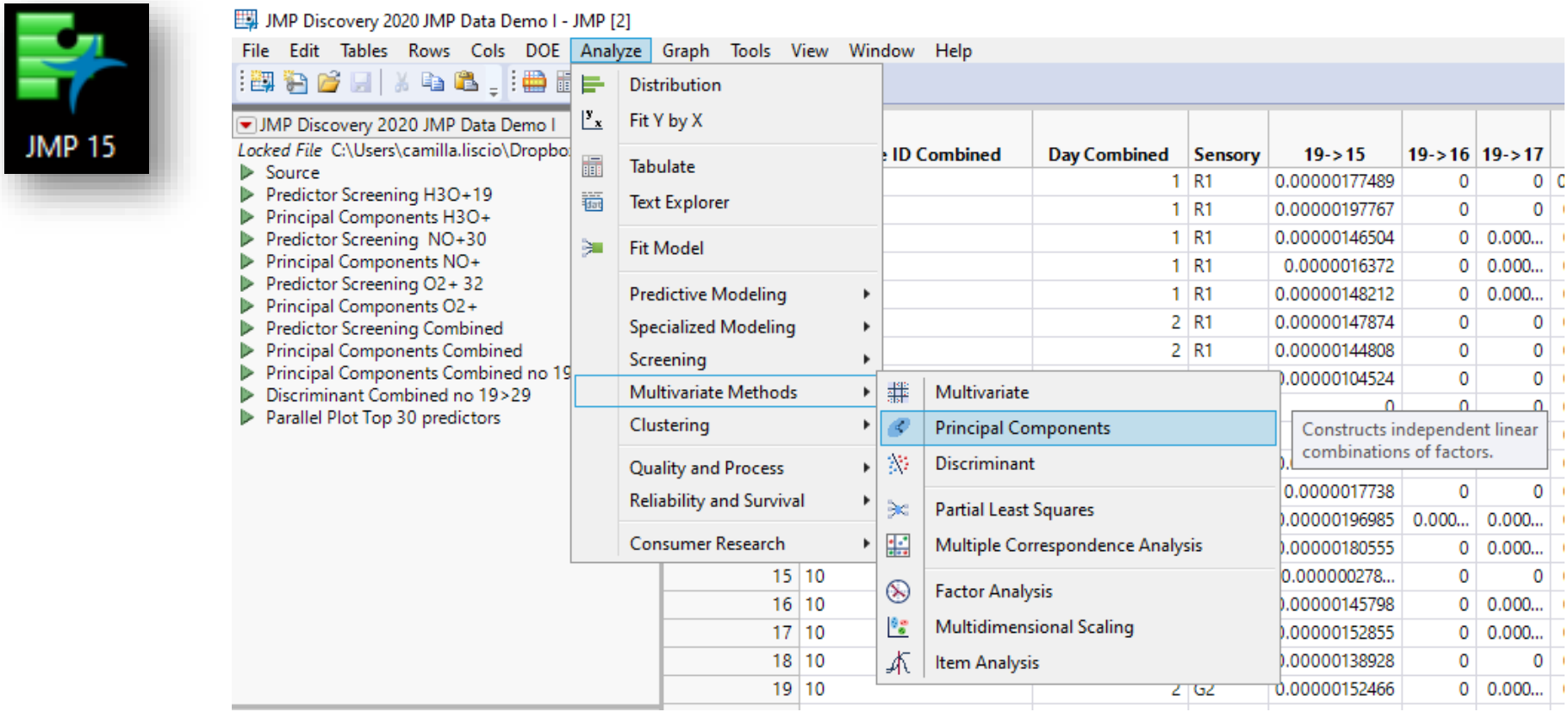


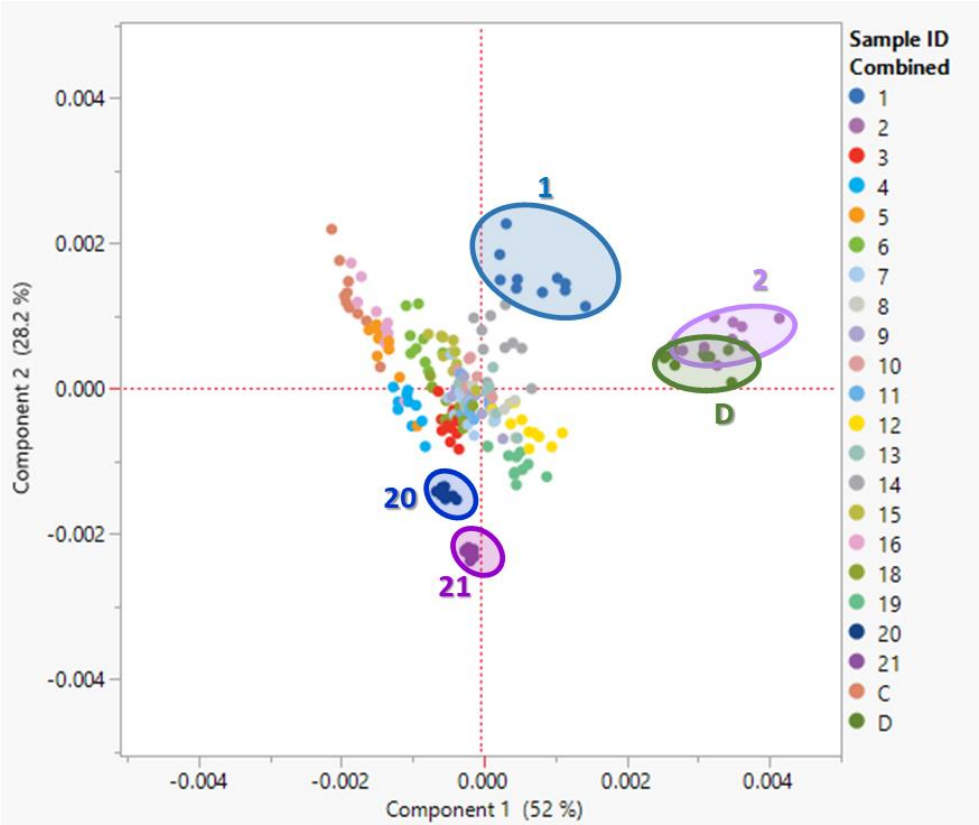


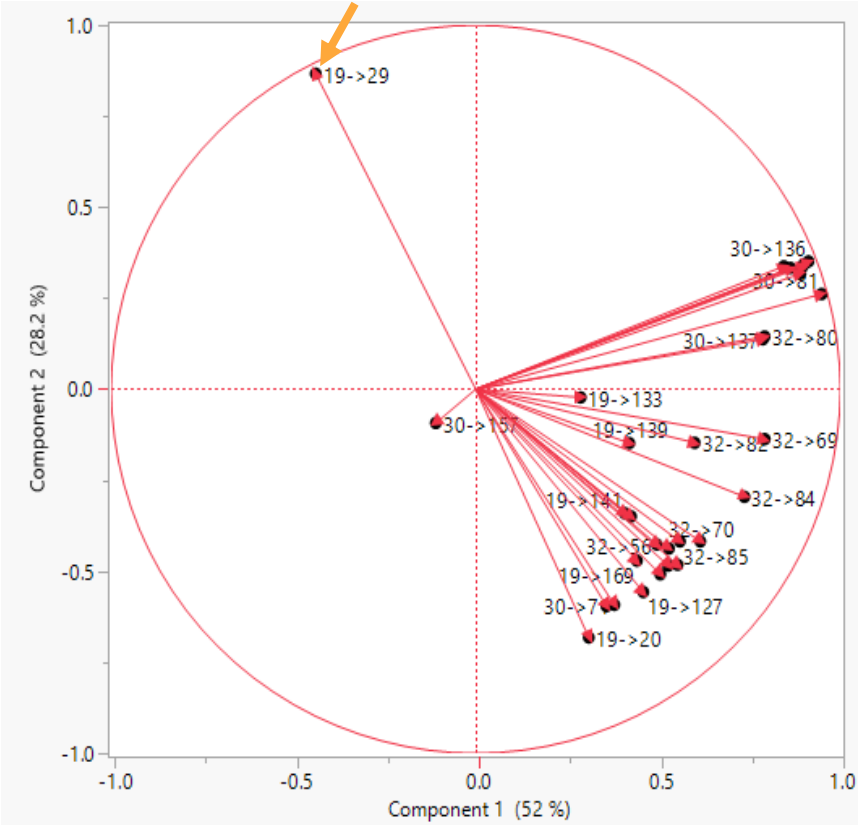
3 Reagent Ions

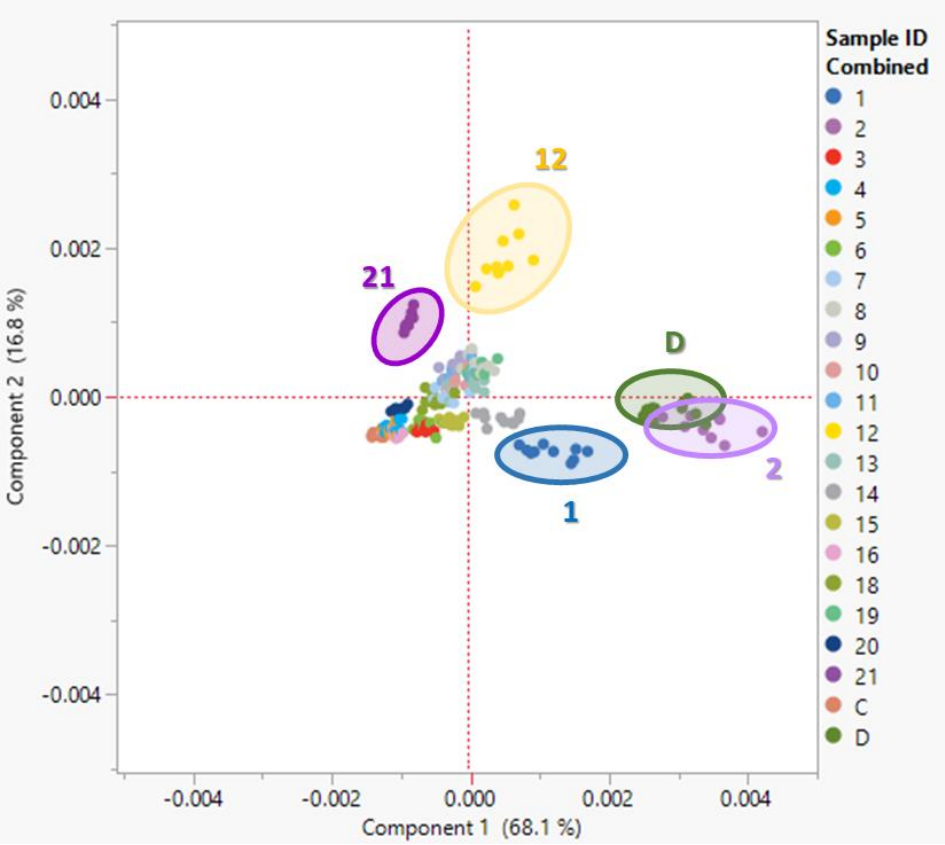
m/z range: 50-250

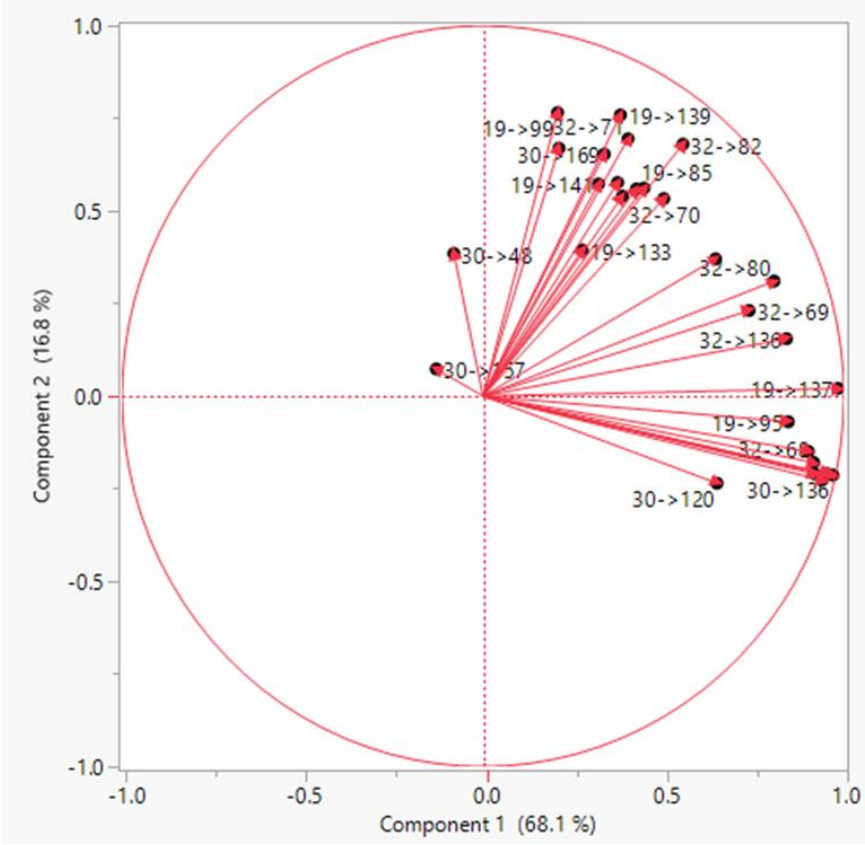

JMP 15

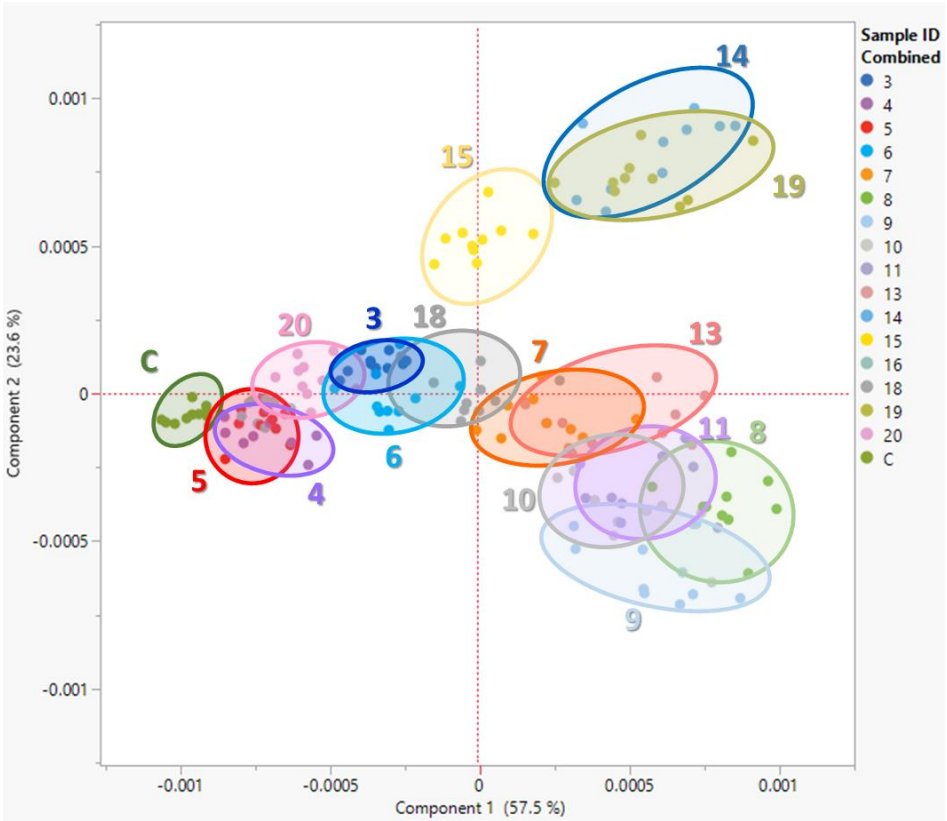

JMP 15
JMP Discovery 2020 JMP Data Demo I - JMP [2]
File Edit Tables Rows Cols DOE Analyze Graph Tools View Window Help
JMP Discovery 2020 JMP Data Demo I
Locked File C:\Users\camilla.liscio\Dropbo
Source
Predictor Screening H3O+19
Principal Components H3O+
Predictor Screening NO+30
Principal Components NO+
Predictor Screening O2+ 32
Principal Components O2+
Predictor Screening Combined
Principal Components Combined
Principal Components Combined no 19
Discriminant Combined no 19>29
Parallel Plot Top 30 predictors
Distribution
Fit Y by X
Tabulate
Text Explorer
Fit Model
Predictive Modeling
Specialized Modeling
Screening
Multivariate Methods
Clustering
Quality and Process
Reliability and Survival
Consumer Research
Multivariate
Principal Components
Discriminant
Partial Least Squares
Multiple Correspondence Analysis
Factor Analysis
Multidimensional Scaling
Item Analysis
Constructs independent linear combinations of factors.
ID Combined
Day Combined
Sensory
19->15
19->16
19->17

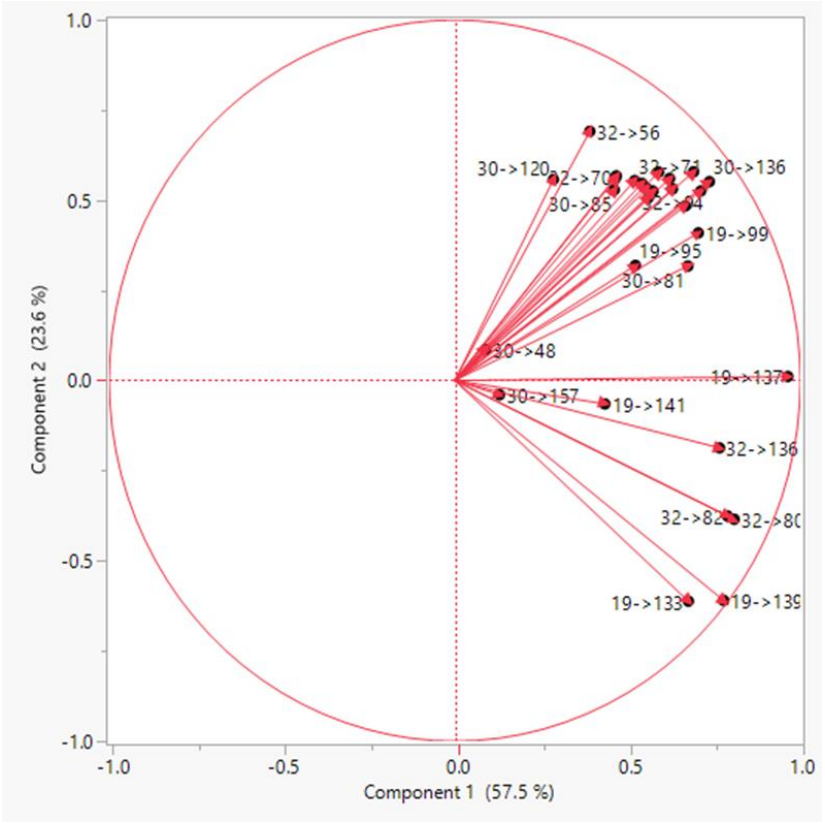

Sample ID Combined
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
18
19
20
21
C
D
1
2
D
20
21
0.004
0.002
0.000
-0.002
-0.004
Component 2 (28.2 %)
-0.004
-0.002
0.000
0.002
0.004
Component 1 (52 %)

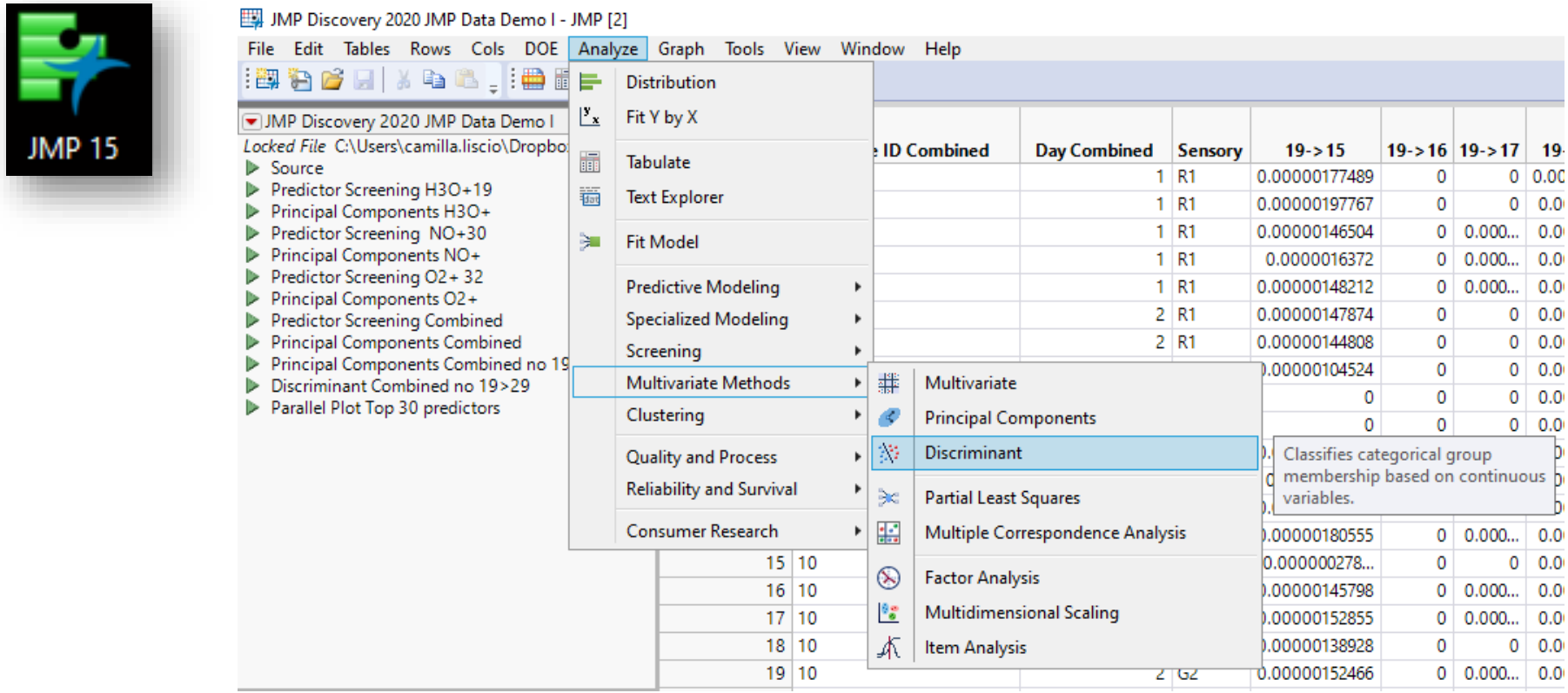

19->29
30->136
30->81
30->137
32->80
19->133
30->157
19->139
32->82
32->69
32->84
19->141
32->70
32->56
32->85
19->169
30->7
19->127
19->20
1.0
0.5
0.0
-0.5
-1.0
Component 2 (28.2 %)
-1.0
-0.5
0.0
0.5
1.0
Component 1 (52 %)


Sample ID Combined
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
18
19
20
21
C
D
12
21
D
2
1
0.004
0.002
0.000
-0.002
-0.004
Component 2 (16.8 %)
-0.004
-0.002
0.000
0.002
0.004
Component 1 (68.1 %)

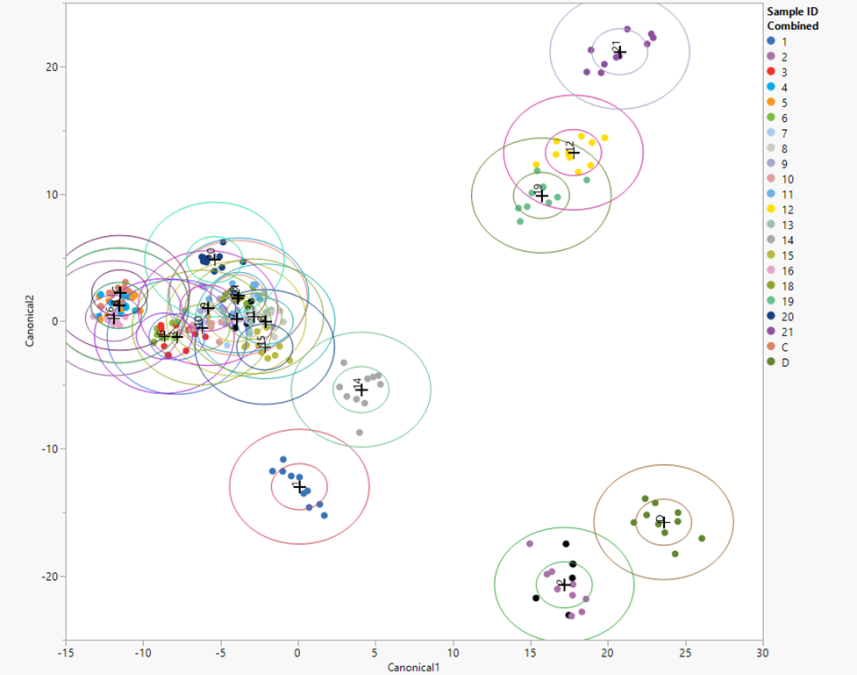

19->99
32->71
19->139
32->82
30->169
19->85
19->141
32->70
30->48
19->133
32->80
32->69
32->136
30->137
19->137
19->95
32->68
30->120
30->136
1.0
0.5
0.0
-0.5
-1.0
Component 2 (16.8 %)
-1.0
-0.5
0.0
0.5
1.0
Component 1 (68.1 %)

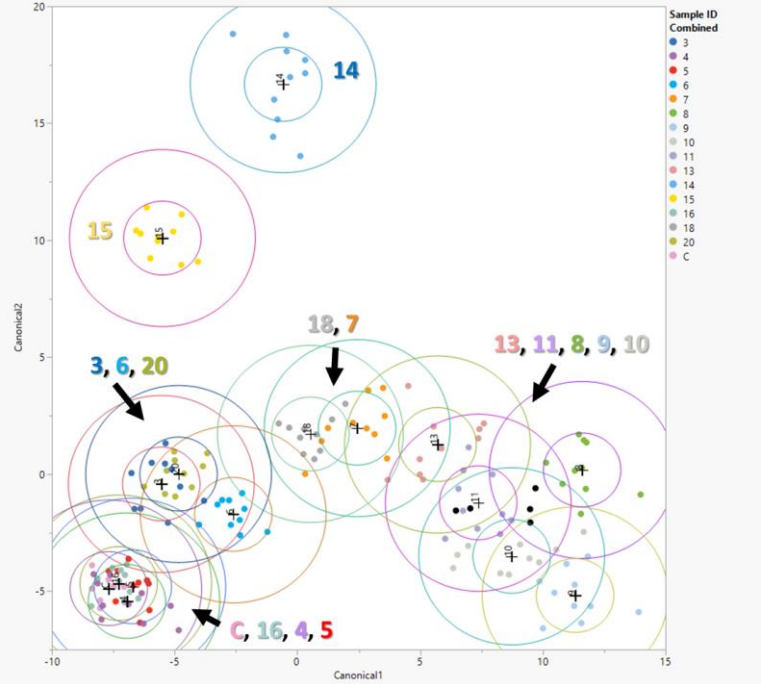

Sample ID
Combined
3
4
5
6
7
8
9
10
11
13
14
15
16
18
19
20
C
14
15
19
20
3
18
C
7
13
5
4
6
11
8
10
9
0.001
0.0005
0
-0.0005
-0.001
Component 2 (23.6 %)
-0.001
-0.0005
0
0.0005
0.001
Component 1 (57.5 %)


32->56
30->120
32->70
30->136
30->85
19->99
19->95
30->81
30->48
19->137
30->157
19->141
32->136
32->82
19->133
1.0
0.5
0.0
-0.5
-1.0
Component 2 (23.6 %)
-1.0
-0.5
0.0
0.5
1.0
Component 1 (57.5 %)


JMP 15
JMP Discovery 2020 JMP Data Demo I - JMP [2]
File Edit Tables Rows Cols DOE Analyze Graph Tools View Window Help
JMP Discovery 2020 JMP Data Demo I
Locked File C:\Users\camilla.liscio\Dropbo
Source
Predictor Screening H3O+19
Principal Components H3O+
Predictor Screening NO+30
Principal Components NO+
Predictor Screening O2+ 32
Principal Components O2+
Predictor Screening Combined
Principal Components Combined
Principal Components Combined no 19
Discriminant Combined no 19>29
Parallel Plot Top 30 predictors
Distribution
Fit Y by X
Tabulate
Text Explorer
Fit Model
Predictive Modeling
Specialized Modeling
Screening
Multivariate Methods
Clustering
Quality and Process
Reliability and Survival
Consumer Research
Multivariate
Principal Components
Discriminant
Partial Least Squares
Multiple Correspondence Analysis
Factor Analysis
Multidimensional Scaling
Item Analysis
Classifies categorical group membership based on continuous variables.
ID Combined
Day Combined
Sensory
19->15
19->16
19->17

Sample No. 5 C	Sample No. 10 Sample No. 9 Sample No. 11 Sample No. 8	Sample No. 6 Sample No. 7 Sample No. 16 Sample No. 18 Sample No. 12 Sample No. 4	Sample No. 19 Sample No. 21	Sample No. 3 Sample No. 14 Sample No. 15	Sample No. 1 Sample No. 2 D	Sample No. 20





Discriminant Scores

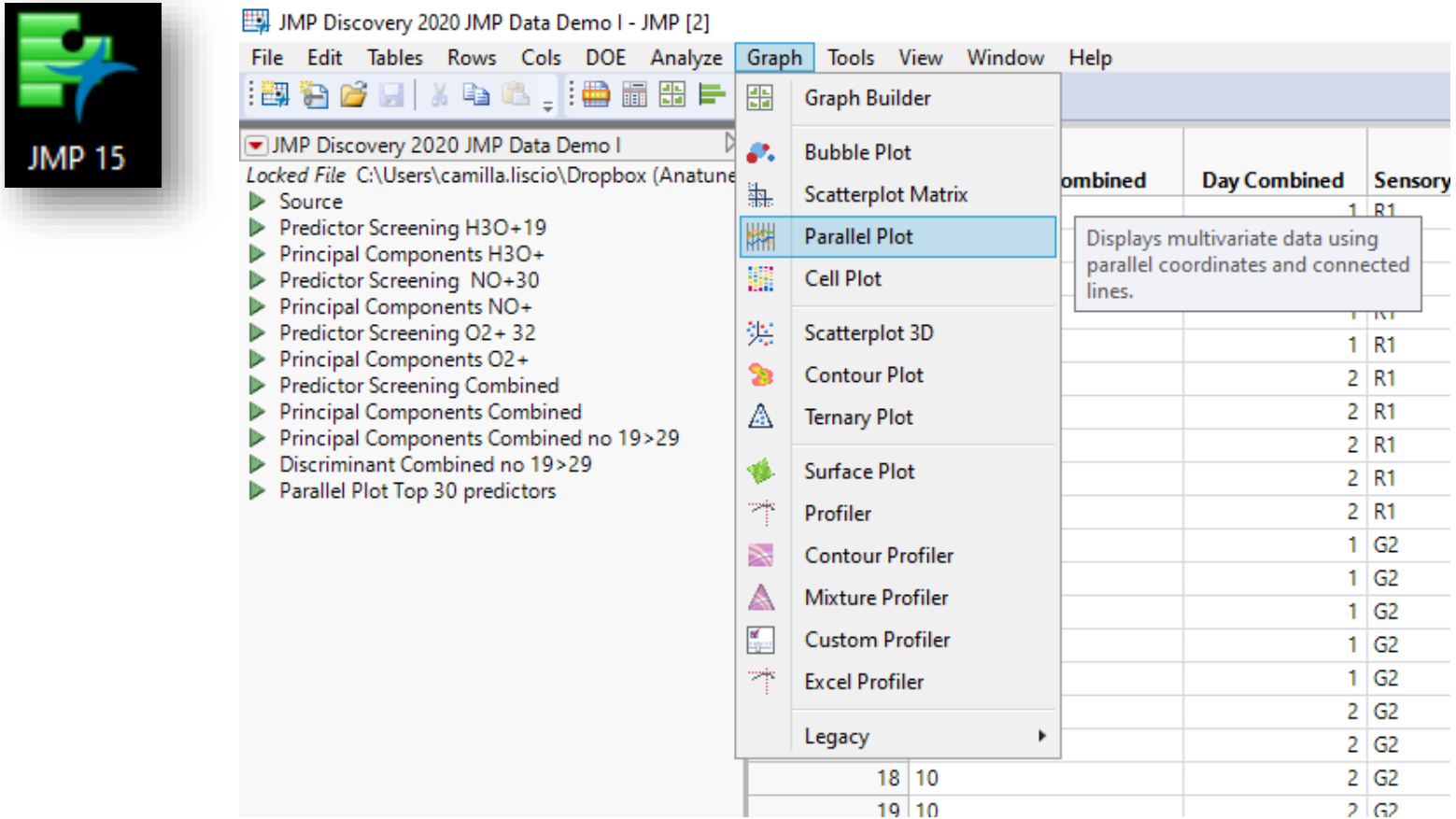
Score Summaries

Source	Count	Number Misclassified	Percent Misclassified	Entropy RSquare	-2LogLikelihood
Training	220	8	3.63636	0.96468	48.0418
Excluded	10	5	50.0000	-4.8245	

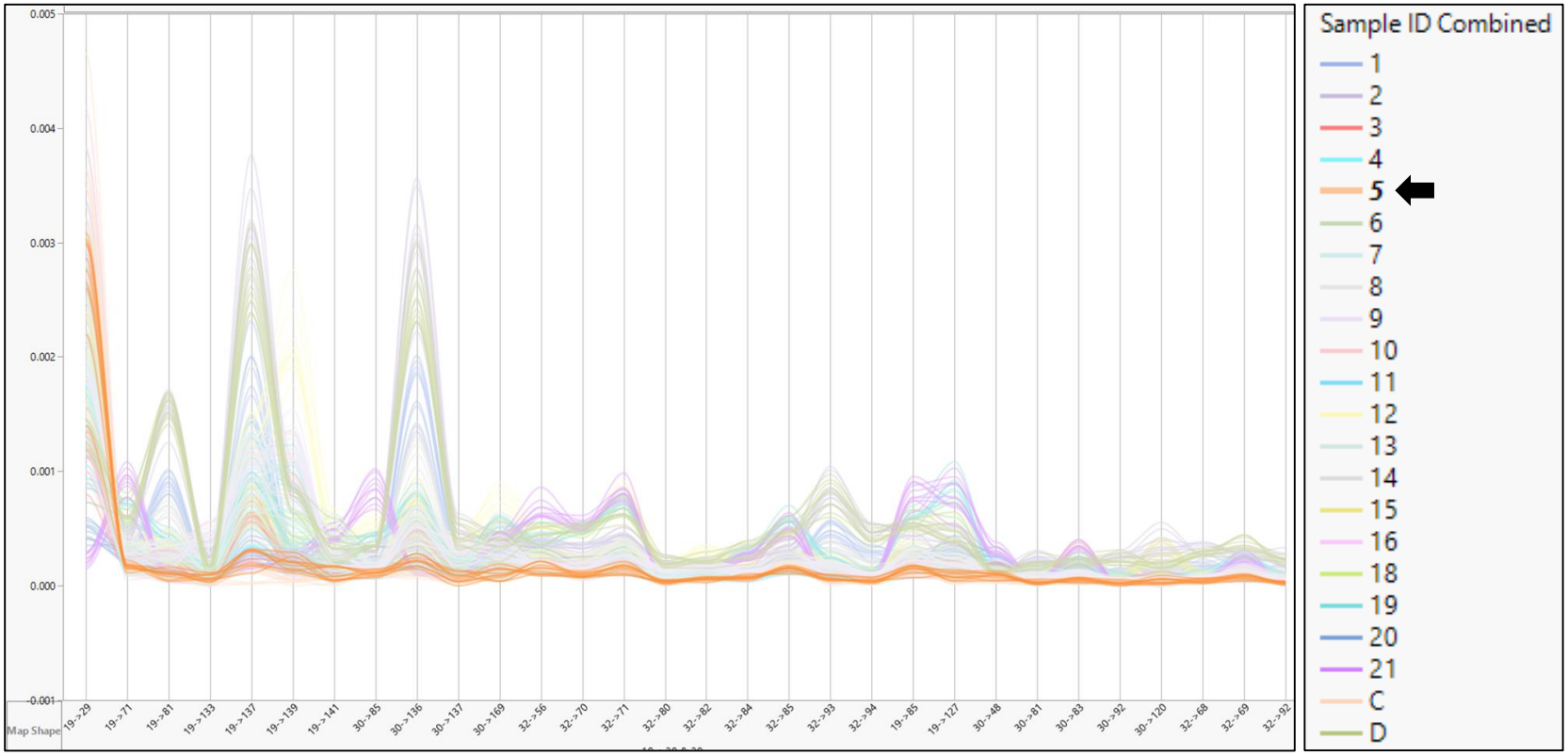
Discriminant Scores

Score Summaries

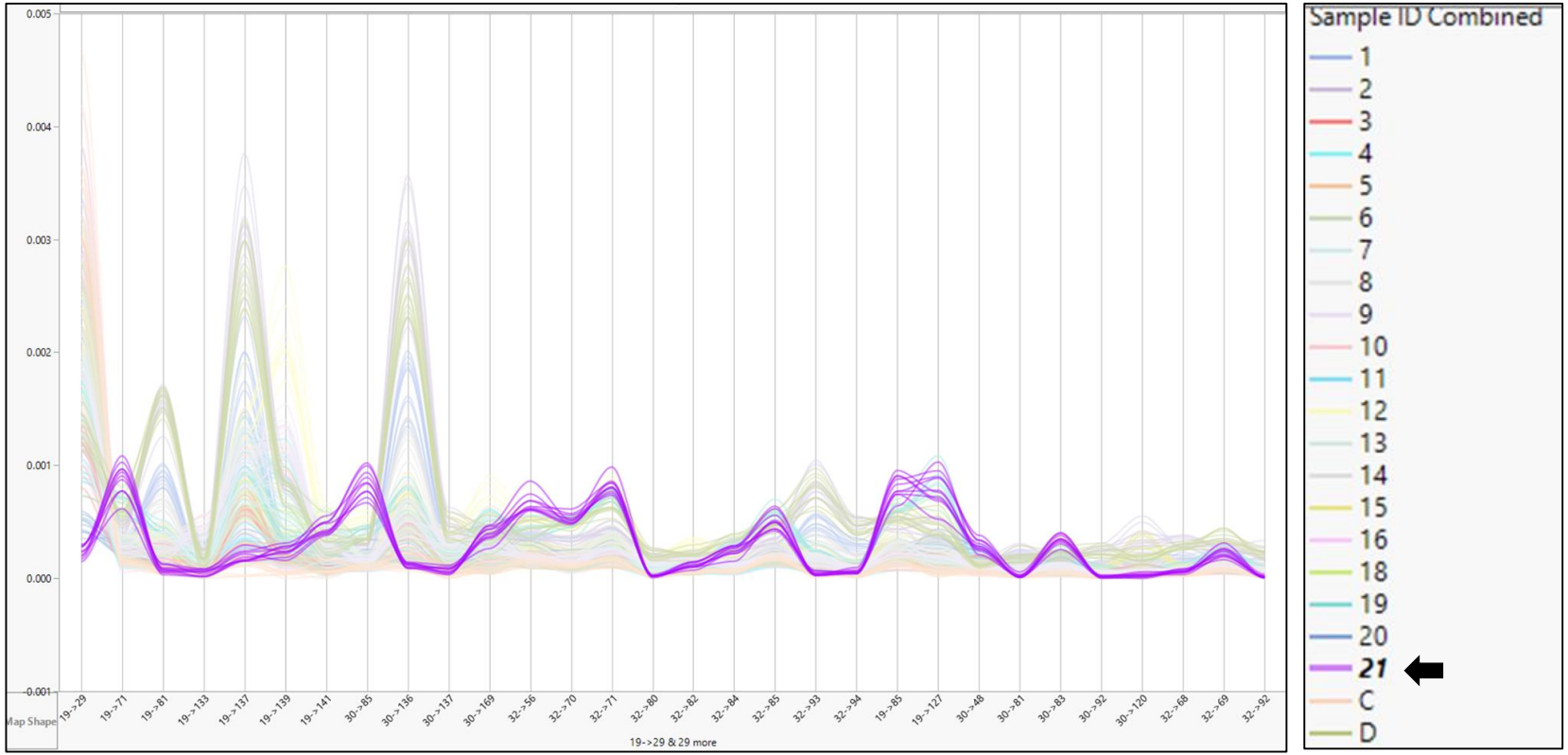
Source	Count	Number Misclassified	Percent Misclassified	Entropy RSquare	-2LogLikelihood
Training	160	2	1.25000	0.97867	18.9237
Excluded	5	4	80.0000	.	


JMP 15
JMP Discovery 2020 JMP Data Demo I - JMP [2]
File Edit Tables Rows Cols DOE Analyze Graph Tools View Window Help
JMP Discovery 2020 JMP Data Demo I
Locked File C:\Users\camilla.liscio\Dropbox (Anatune
Source
Predictor Screening H3O+19
Principal Components H3O+
Predictor Screening NO+30
Principal Components NO+
Predictor Screening O2+ 32
Principal Components O2+
Predictor Screening Combined
Principal Components Combined
Principal Components Combined no 19>29
Discriminant Combined no 19>29
Parallel Plot Top 30 predictors
Graph Builder
Bubble Plot
Scatterplot Matrix
Parallel Plot
Cell Plot
Scatterplot 3D
Contour Plot
Ternary Plot
Surface Plot
Profiler
Contour Profiler
Mixture Profiler
Custom Profiler
Excel Profiler
Legacy
Displays multivariate data using parallel coordinates and connected lines.
ombined
Day Combined
Sensory
1 R1
1 R1
2 R1
2 R1
2 R1
2 R1
2 R1
1 G2
1 G2
1 G2
1 G2
1 G2
2 G2
2 G2
18 10
2 G2
19 10
2 G2

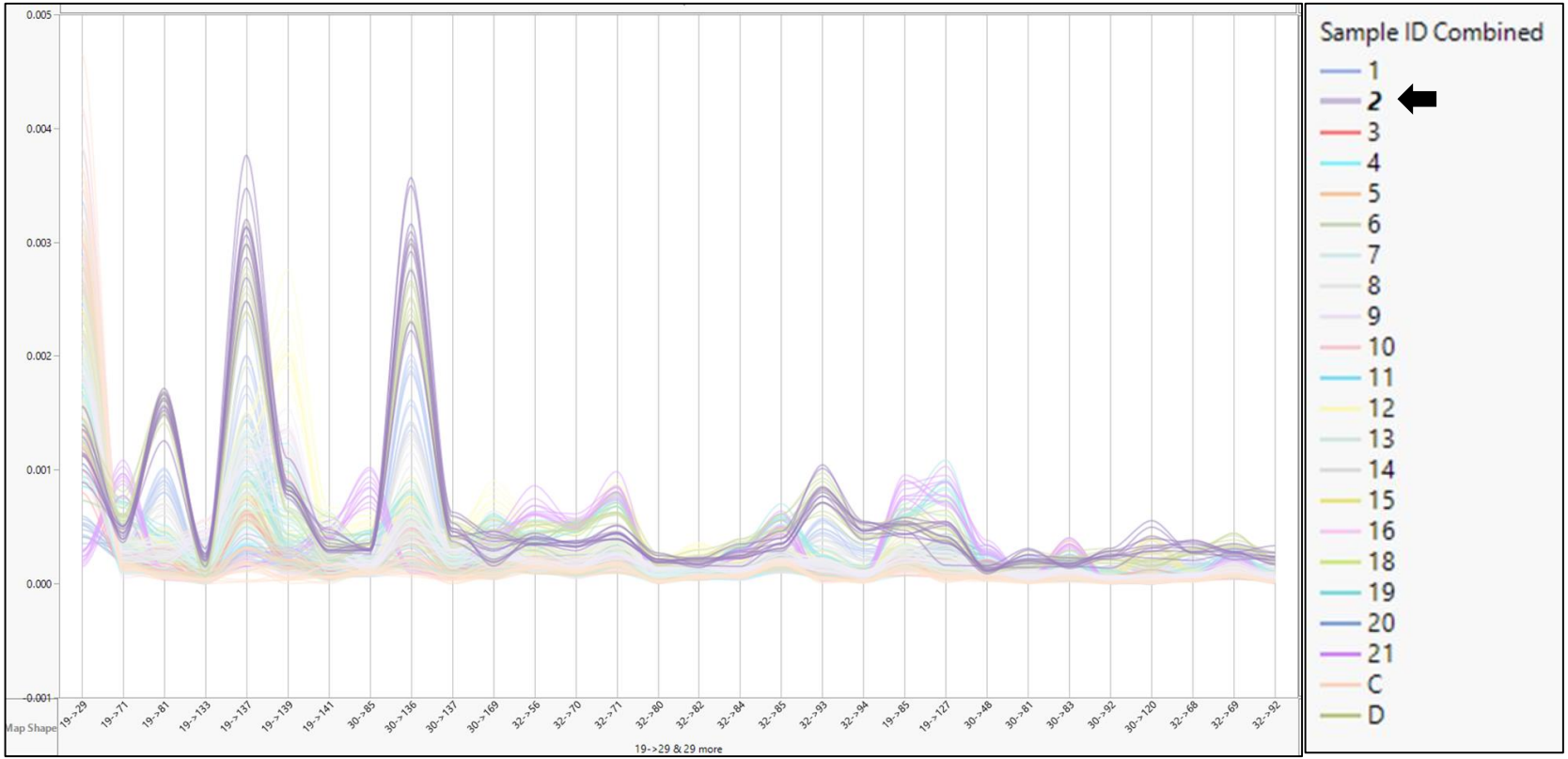
Sample No. 5 C	Sample No. 10 Sample No. 9 Sample No. 11 Sample No. 8	Sample No. 6 Sample No. 7 Sample No. 16 Sample No. 18 Sample No. 12 Sample No. 4	Sample No. 19 Sample No. 21	Sample No. 3 Sample No. 14 Sample No. 15	Sample No. 1 Sample No. 2 D	Sample No. 20



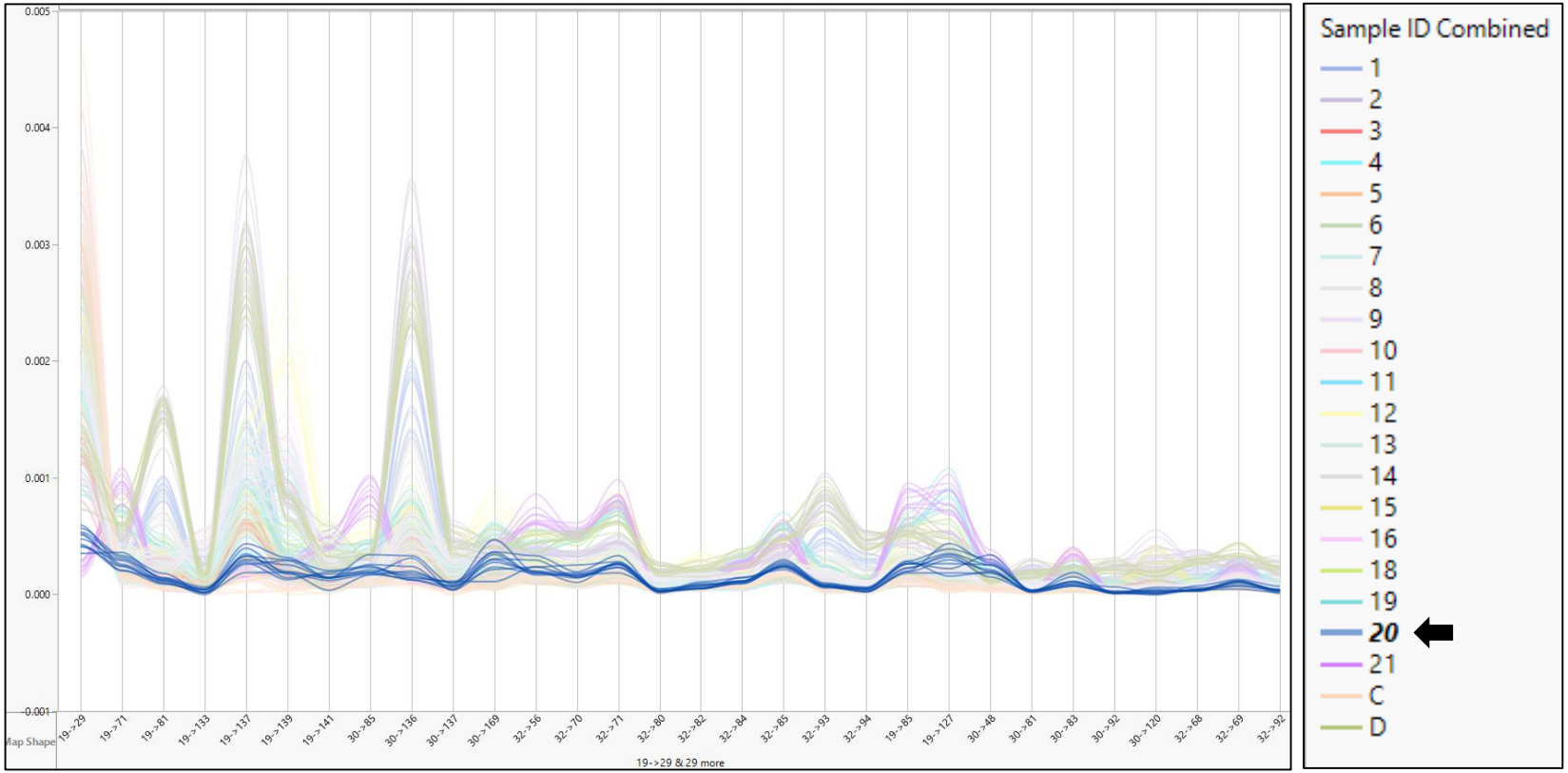
Sample No. 5 C	Sample No. 10 Sample No. 9 Sample No. 11 Sample No. 8	Sample No. 6 Sample No. 7 Sample No. 16 Sample No. 18 Sample No. 12 Sample No. 4	Sample No. 19 Sample No. 21	Sample No. 3 Sample No. 14 Sample No. 15	Sample No. 1 Sample No. 2 D	Sample No. 20

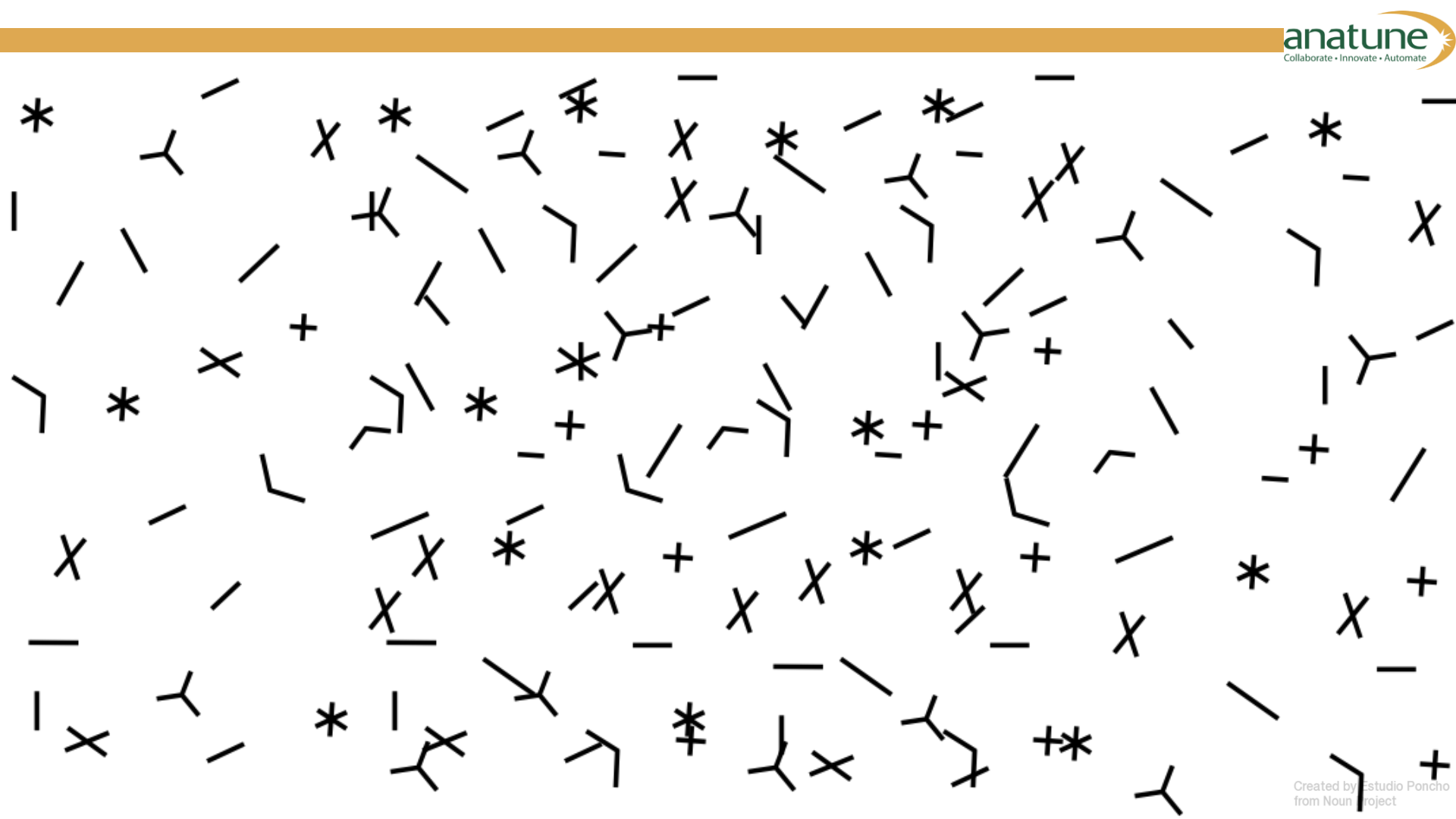


Sample No. 5 C	Sample No. 10 Sample No. 9 Sample No. 11 Sample No. 8	Sample No. 6 Sample No. 7 Sample No. 16 Sample No. 18 Sample No. 12 Sample No. 4	Sample No. 19 Sample No. 21	Sample No. 3 Sample No. 14 Sample No. 15	Sample No. 1 Sample No. 2 D	Sample No. 20



Sample No. 5 C	Sample No. 10 Sample No. 9 Sample No. 11 Sample No. 8	Sample No. 6 Sample No. 7 Sample No. 16 Sample No. 18 Sample No. 12 Sample No. 4	Sample No. 19 Sample No. 21	Sample No. 3 Sample No. 14 Sample No. 15	Sample No. 1 Sample No. 2 D	Sample No. 20

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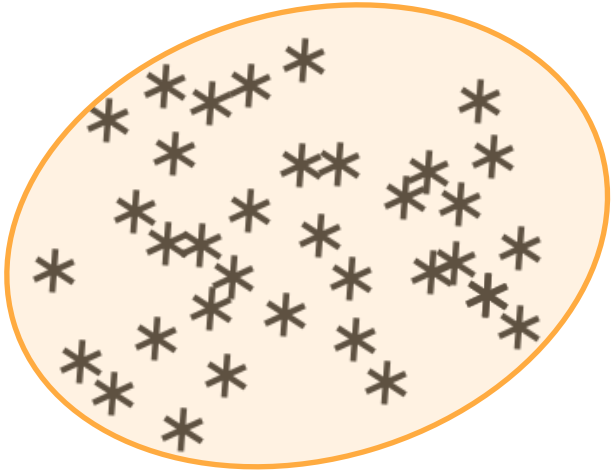
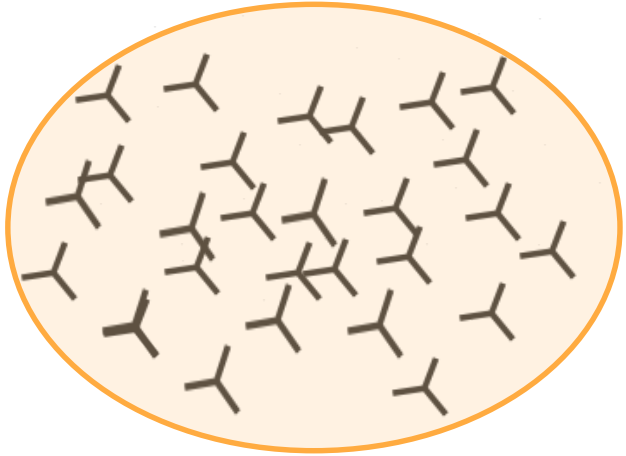
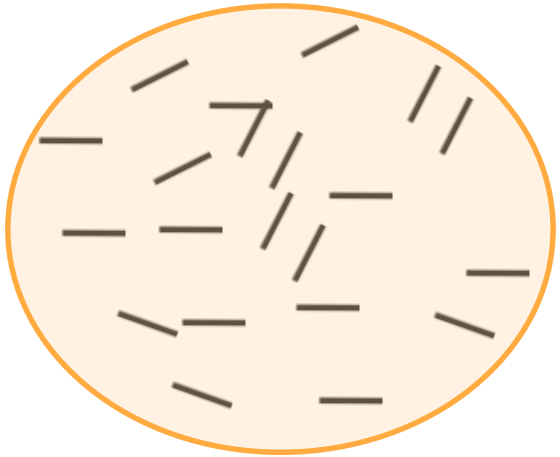
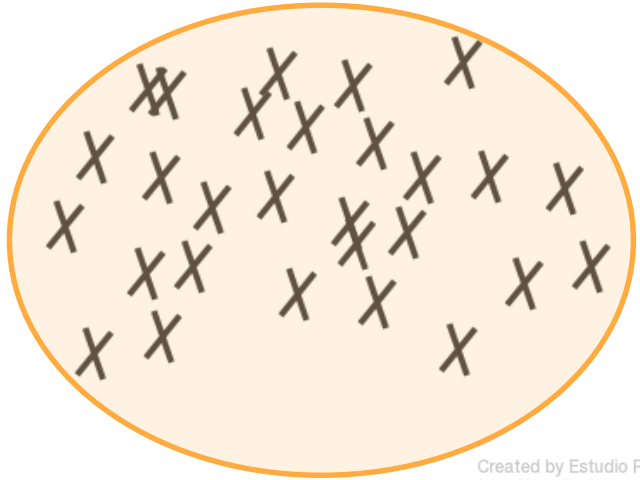
from Noun Project





DATA ANALYTICS





"Out of complexity, find simplicity"

A. Einstein

Thanks to

Our customers

The Anatune Team

Phil Kay, JMP

camilla.liscio@anatune.co.uk

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enquiries@anatune.co.uk
01223 279 210