Improving Gas Chromatography/Vacuum Ultraviolet Spectroscopy (GC/VUV) for Forensic Science using JMP

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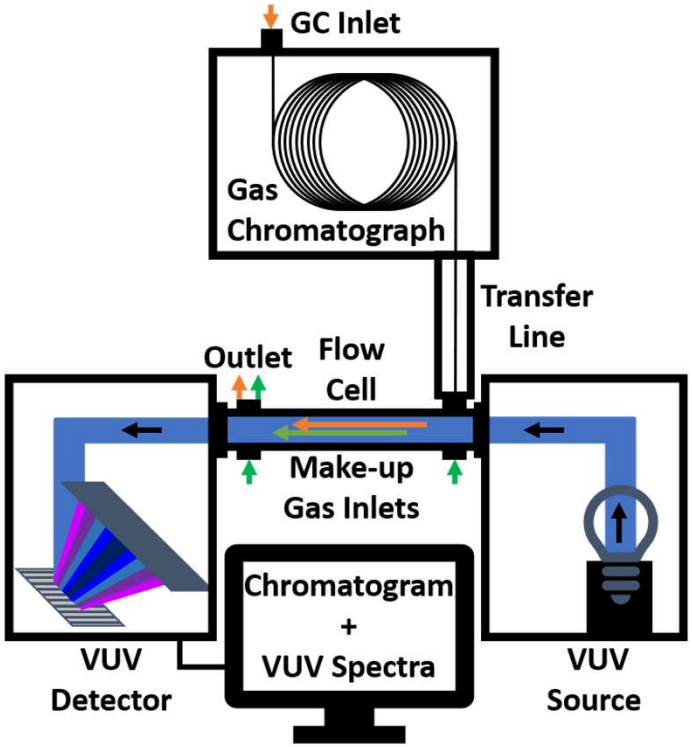
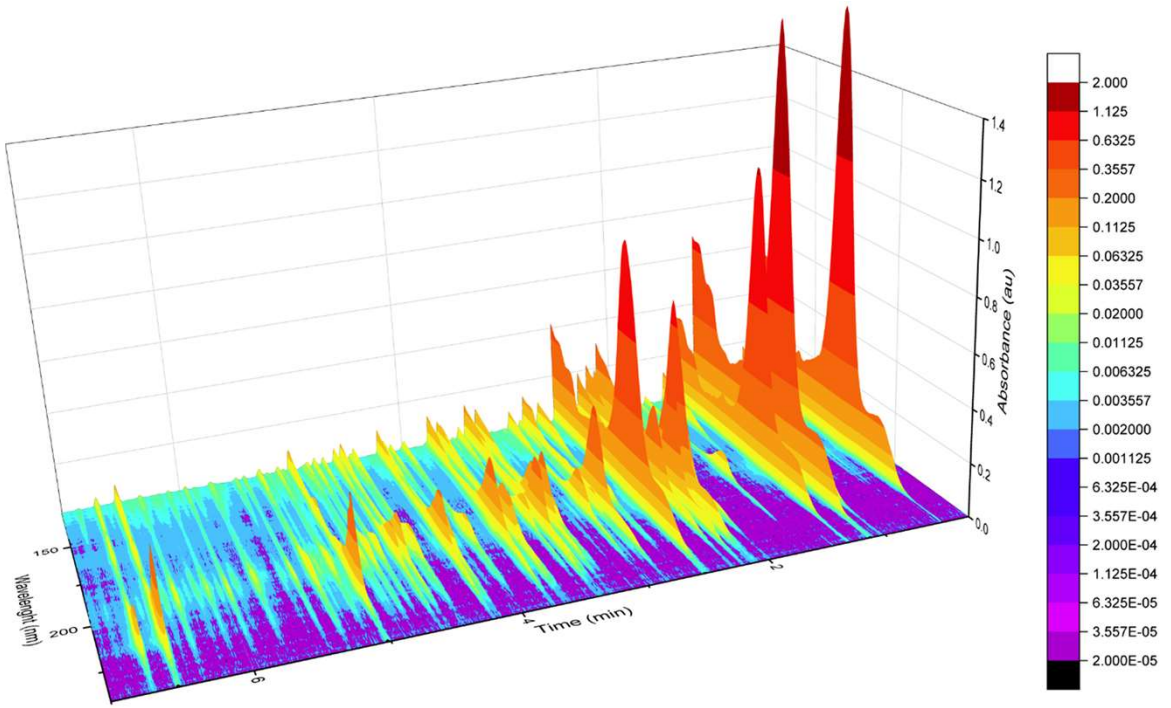
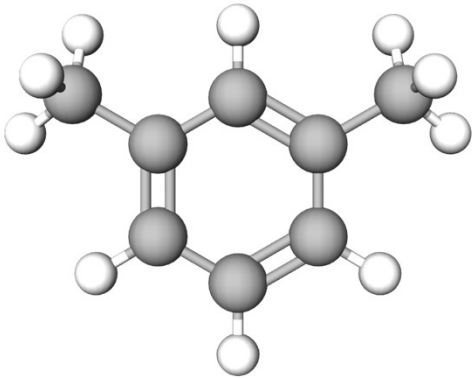
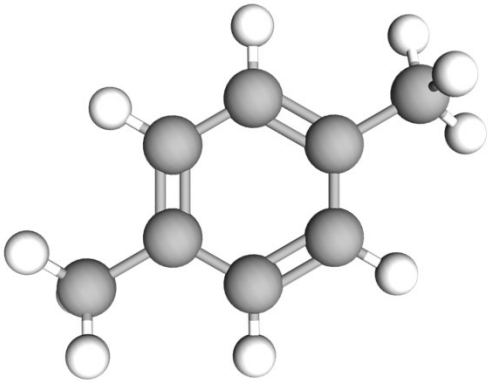

GC Inlet
Gas
Chromatograph
Transfer
Line
Outlet
Flow
Cell
Make-up
Gas Inlets
Chromatogram
+
VUV Spectra
VUV
Detector
VUV
Source


Wavelength (nm)
150
200
Time (min)
Absorbance (au)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
2.000
1.125
0.6325
0.3557
0.2000
0.1125
0.06325
0.03557
0.02000
0.01125
0.006325
0.003557
0.002000
0.001125
6.325E-04
3.557E-04
2.000E-04
1.125E-04
6.325E-05
3.557E-05
2.000E-05

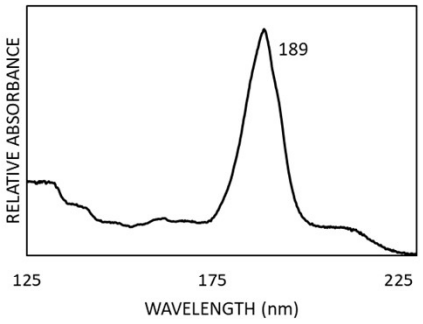


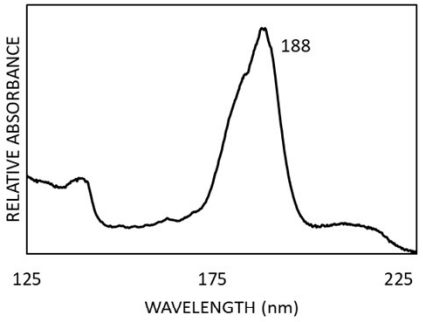
1,3-Dimethybenzene

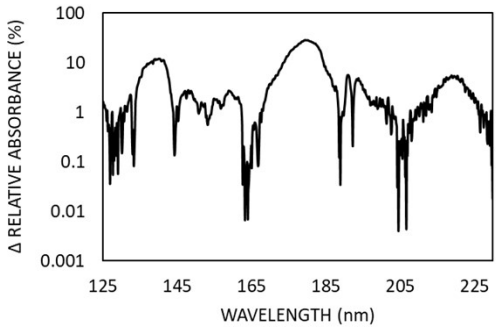


1,4-Dimethybenzene

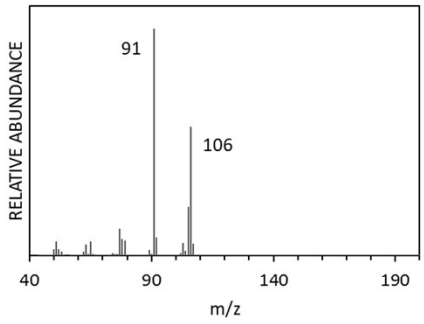
VUV Spectrum

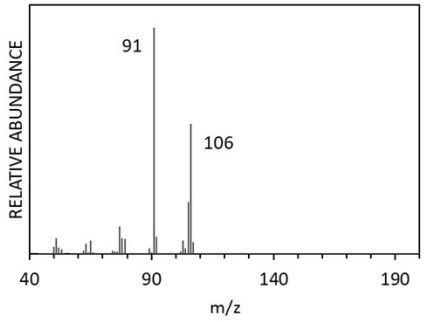


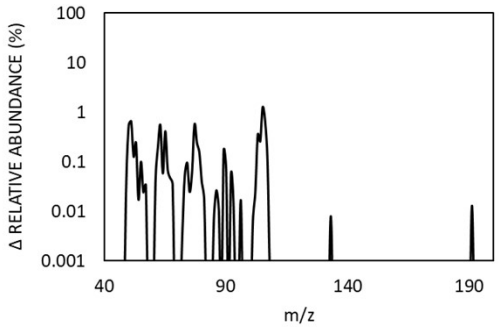




Mass Spectrum







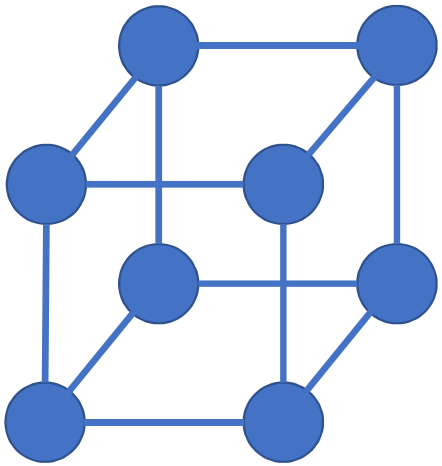
Method Development and Optimization

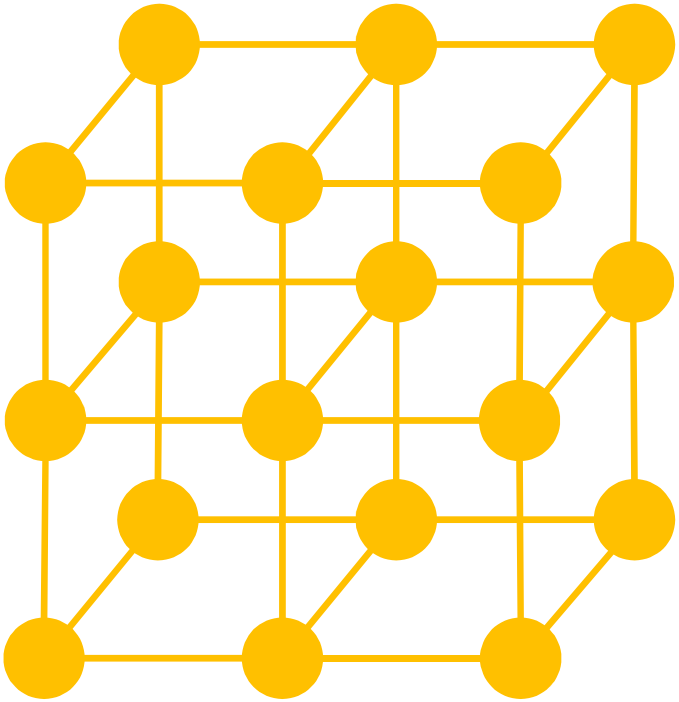
Full Factorials and Response Surfaces

Full Factorial

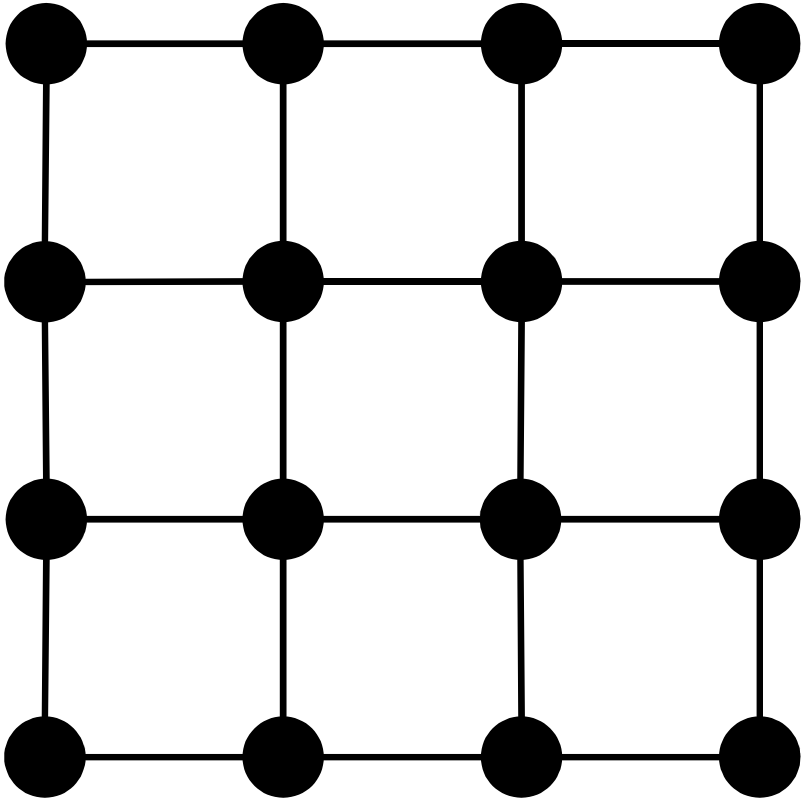
- n Factors
- n Levels

3 Factor; 2 Level





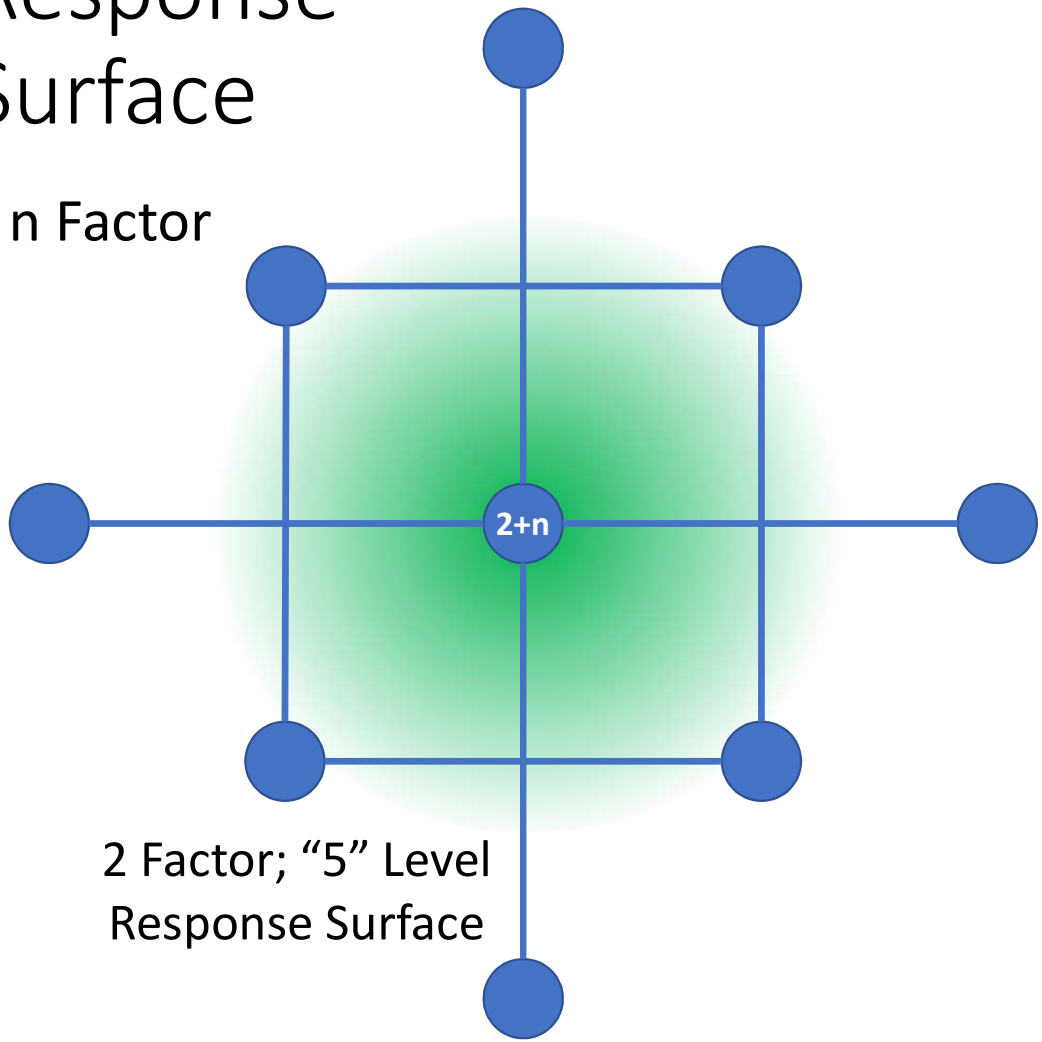
3 Factor; 3, 3, 2 Level



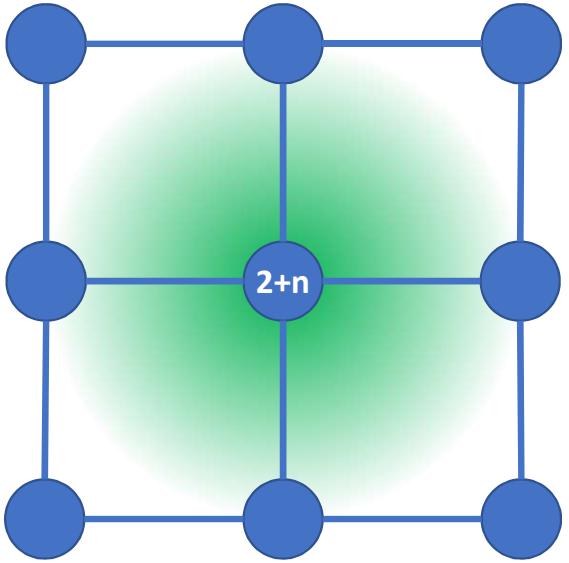
2 Factor; 4 Level

Response Surface

- n Factor



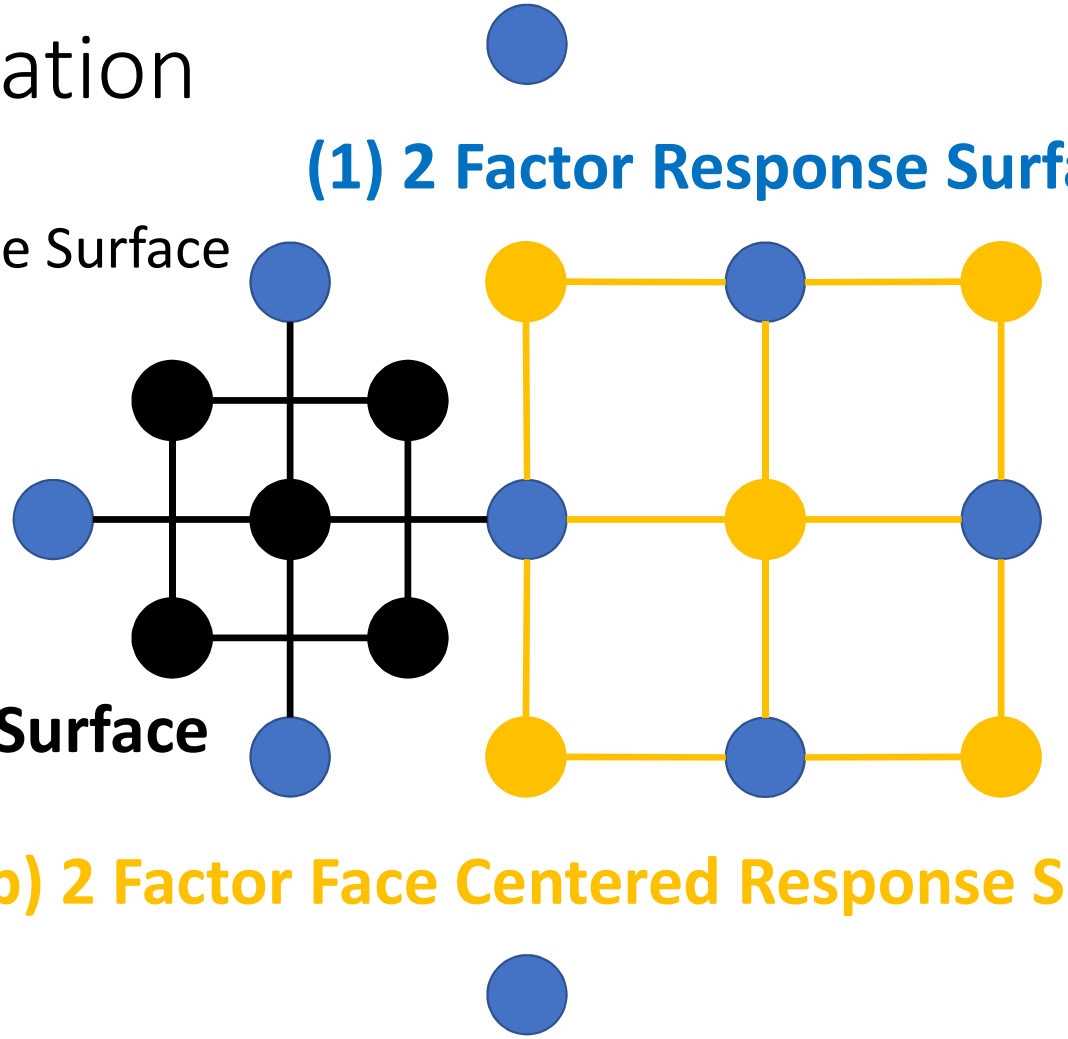
2 Factor; “5” Level
Response Surface



2 Factor; 3 Level
Face Centered Response Surface

Iterative Optimization

- Full Factorial or Response Surface
- n Factor
- n Iterations

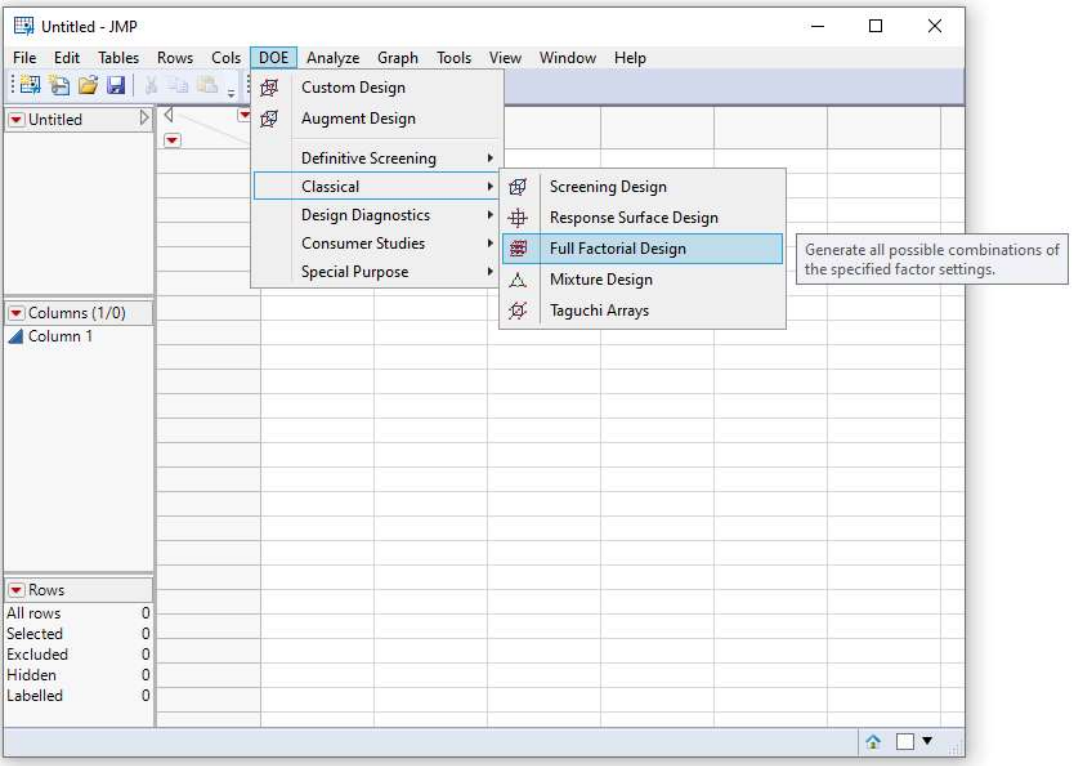


(1) 2 Factor Response Surface

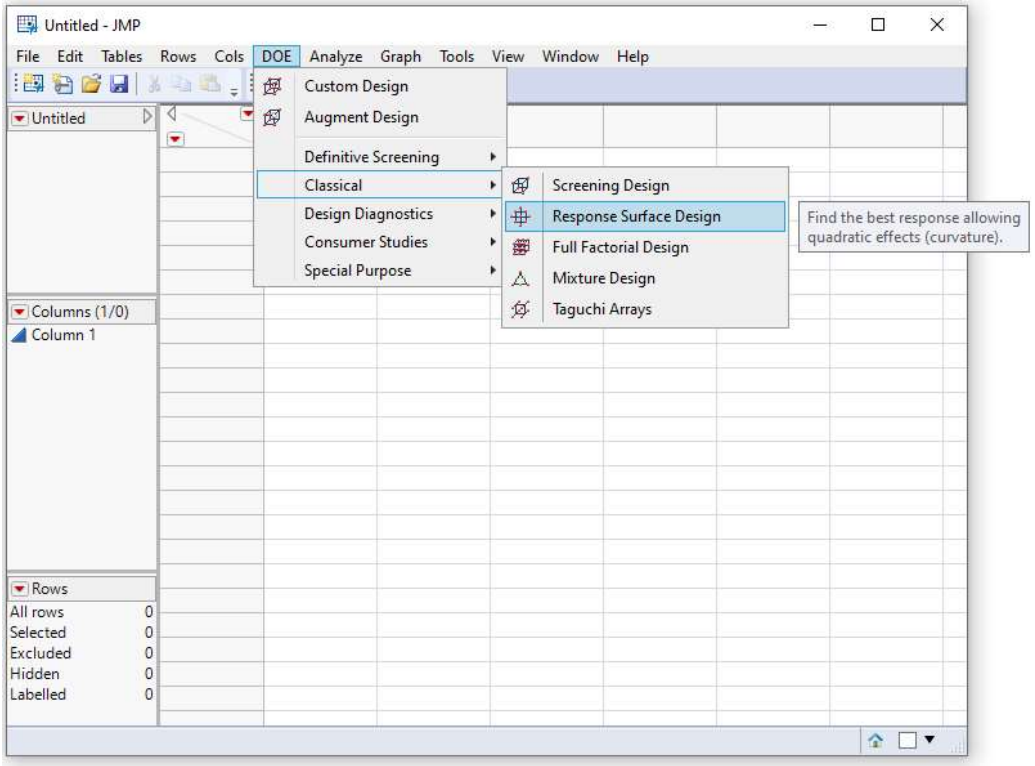
(2a) 2 Factor Response Surface

(2b) 2 Factor Face Centered Response Surface

Full Factorial



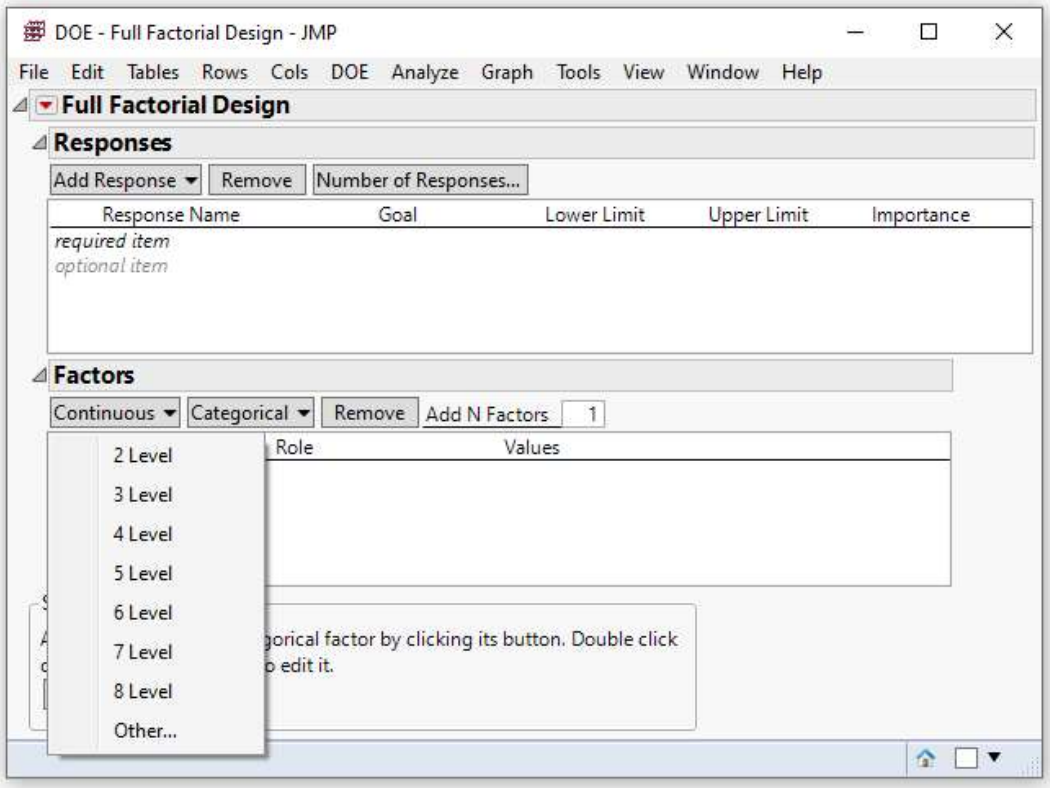
Response Surface

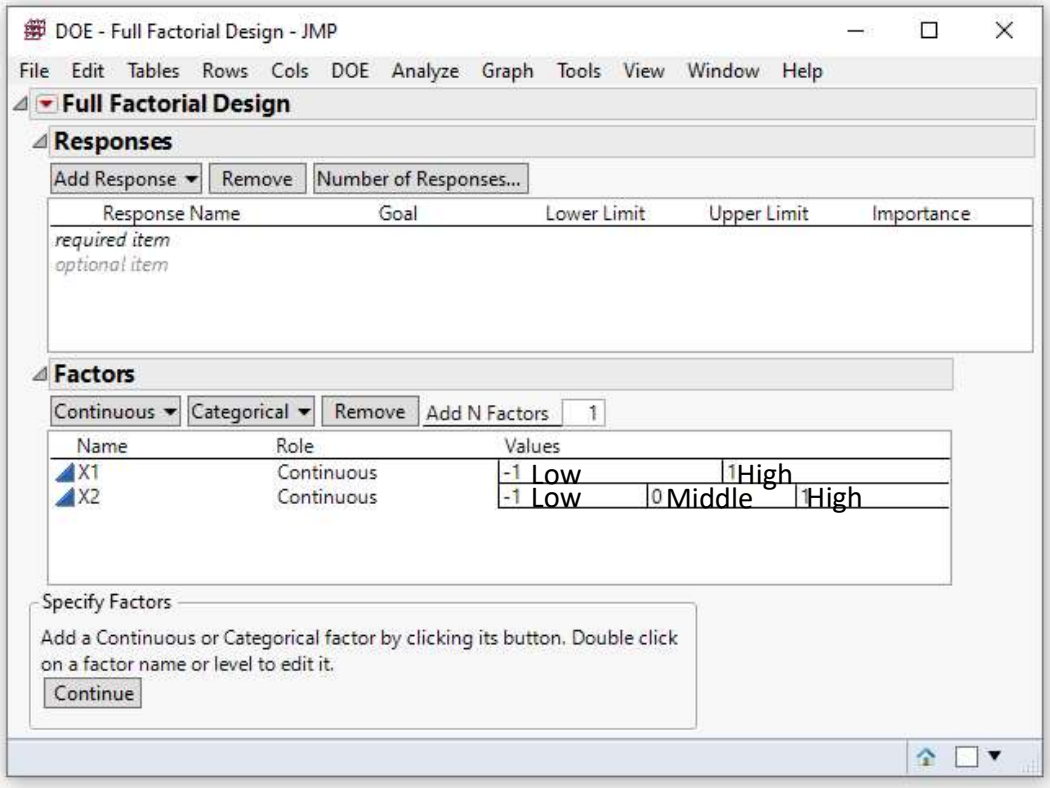


Full Factorial

Factors

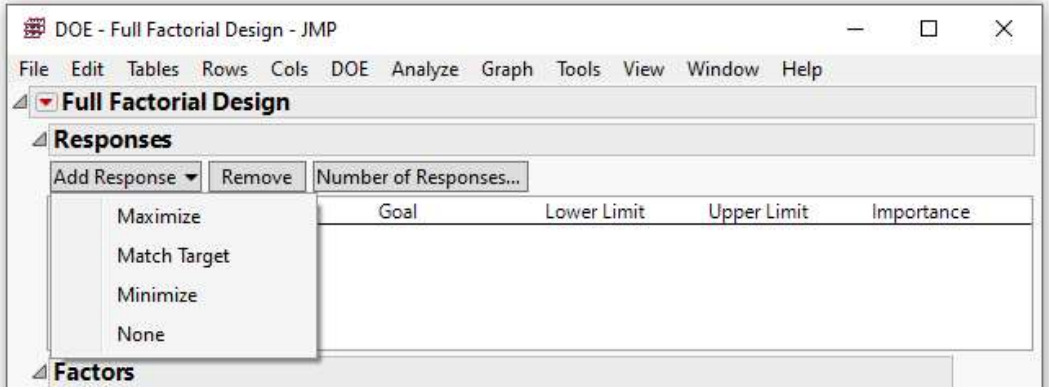
Levels



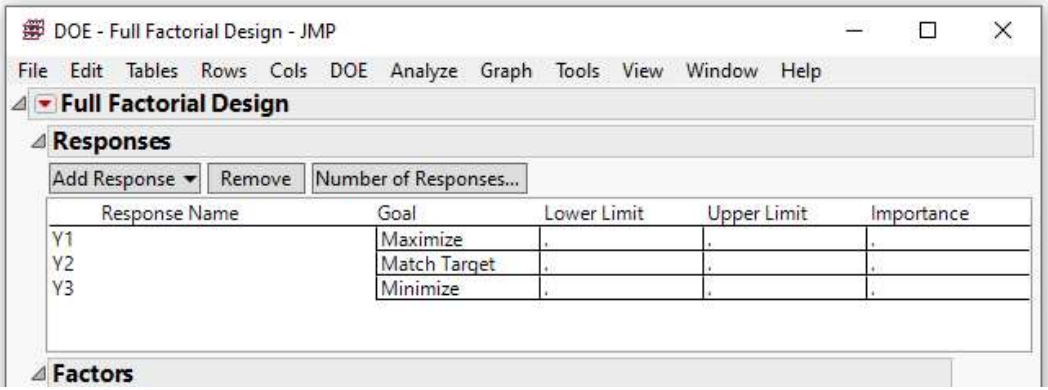


Full Factorial

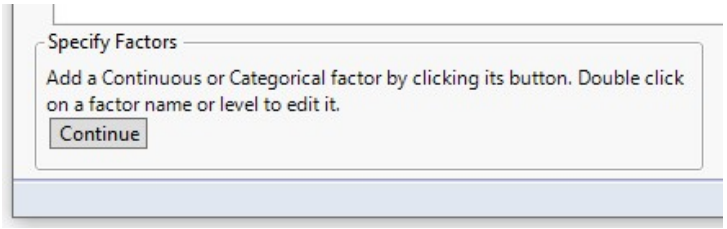
Responses

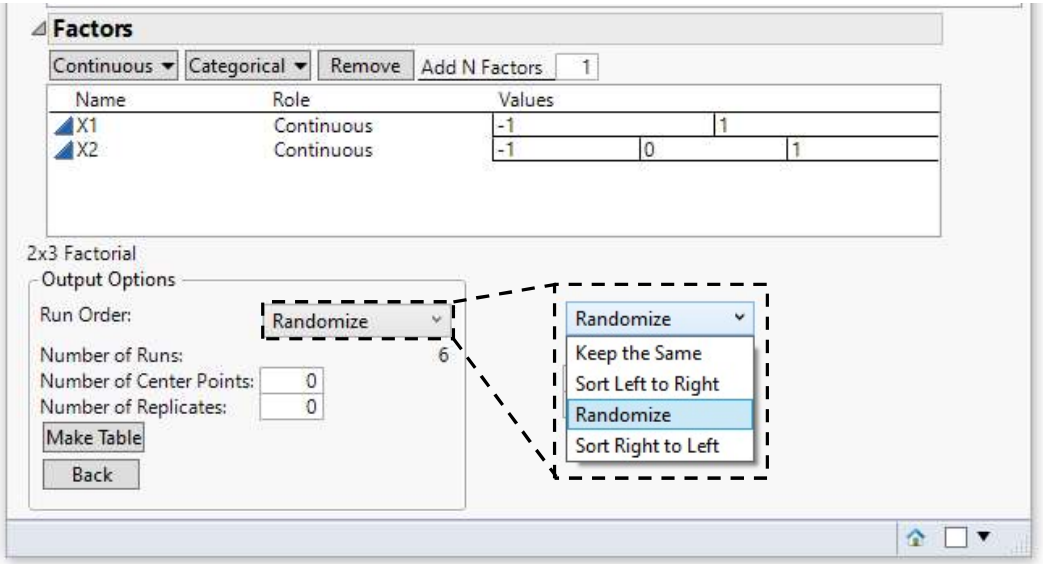


Desirability Contributions

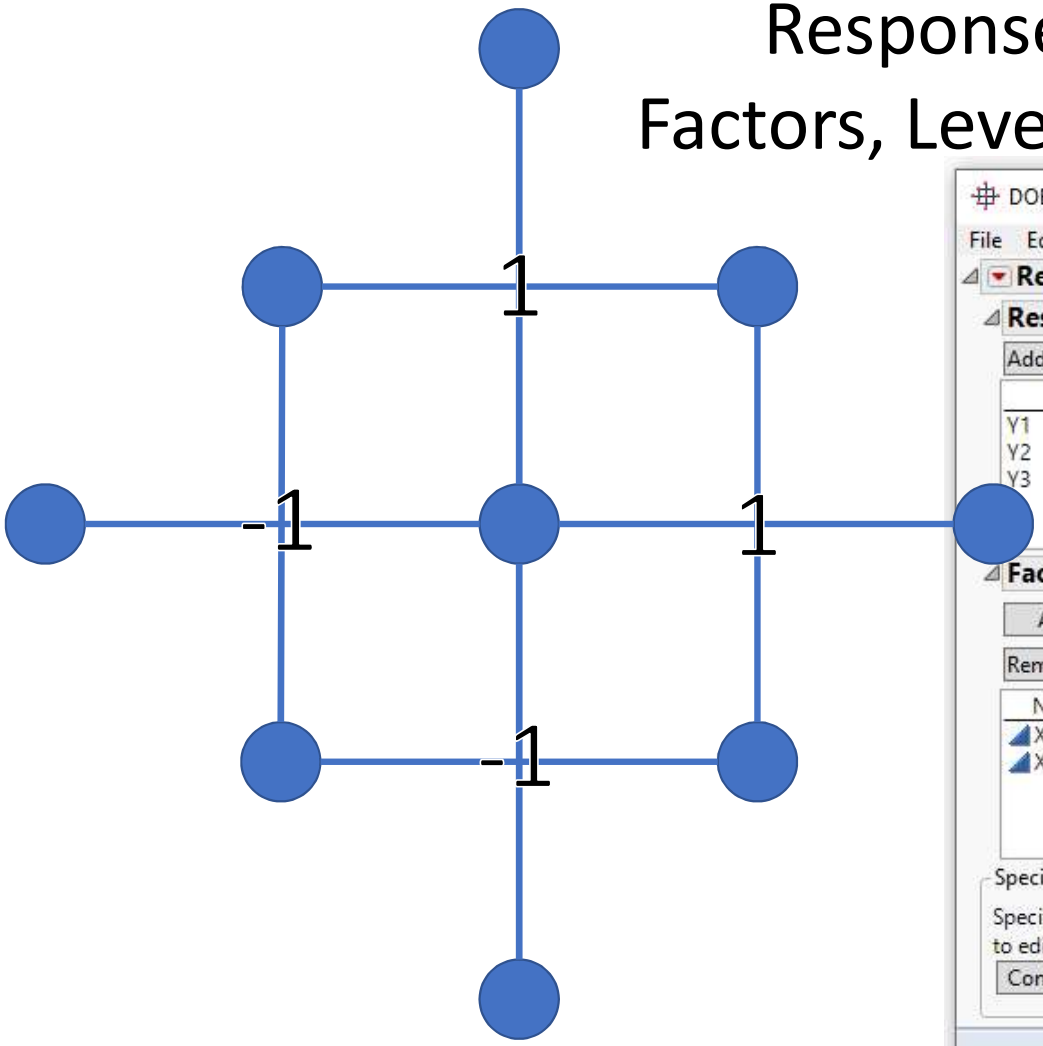


Full Factorial:
Run Order, Center Points, Replicates





Response Surface:
Factors, Levels, Responses



DOE - Response Surface Design - JMP

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

Response Surface Design

Responses

Add Response | Remove | Number of Responses...

Response Name	Goal	Lower Limit	Upper Limit	Importance
Y1	Maximize	.	.	.
Y2	Match Target	.	.	.
Y3	Minimize	.	.	.

Factors

Add 1 Continuous

Remove Selected

Name	Role	Values	
X1	Continuous	-1	1
X2	Continuous	-1	1

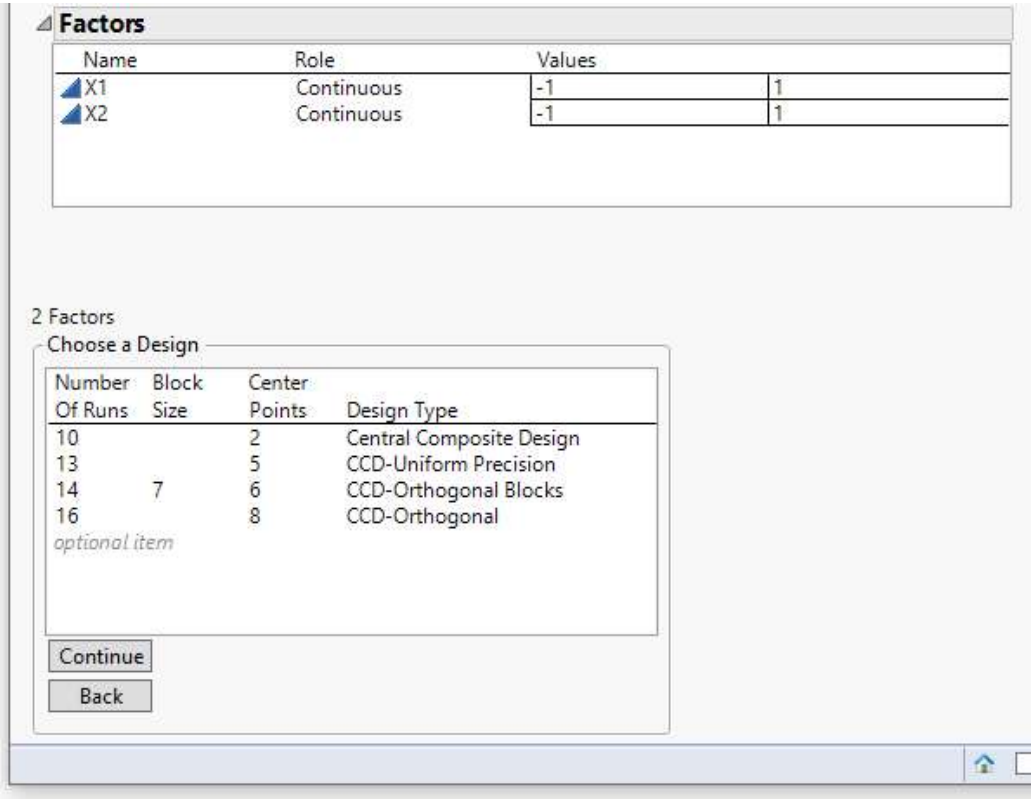
Specify Factors

Specify desired number of factors. Double click on a factor name or setting to edit it.

Continue

Response Surface:
Designs

2 Factor



Factors

Name	Role	Values	
X1	Continuous	-1	1
X2	Continuous	-1	1

2 Factors

Choose a Design

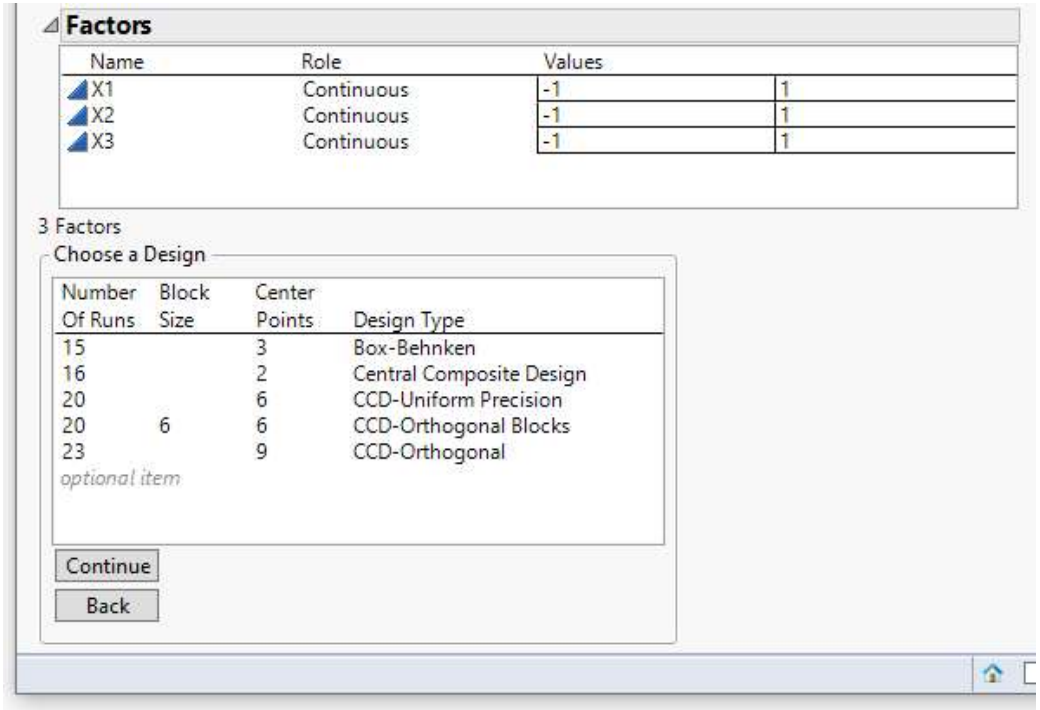
Number Of Runs	Block Size	Center Points	Design Type
10		2	Central Composite Design
13		5	CCD-Uniform Precision
14	7	6	CCD-Orthogonal Blocks
16		8	CCD-Orthogonal

optional item

Continue

Back

3 Factor



Factors

Name	Role	Values	
X1	Continuous	-1	1
X2	Continuous	-1	1
X3	Continuous	-1	1

3 Factors

Choose a Design

Number Of Runs	Block Size	Center Points	Design Type
15		3	Box-Behnken
16		2	Central Composite Design
20		6	CCD-Uniform Precision
20	6	6	CCD-Orthogonal Blocks
23		9	CCD-Orthogonal

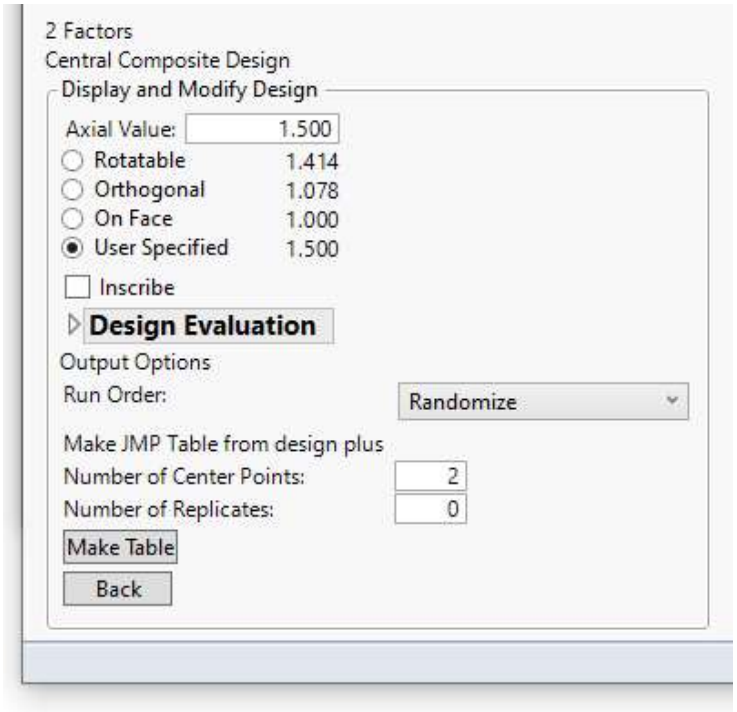
optional item

Continue

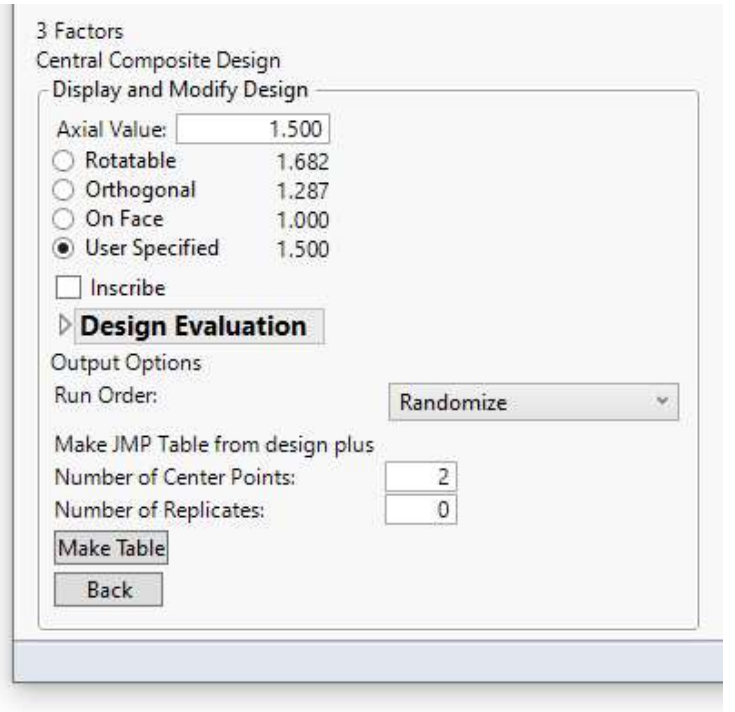
Back

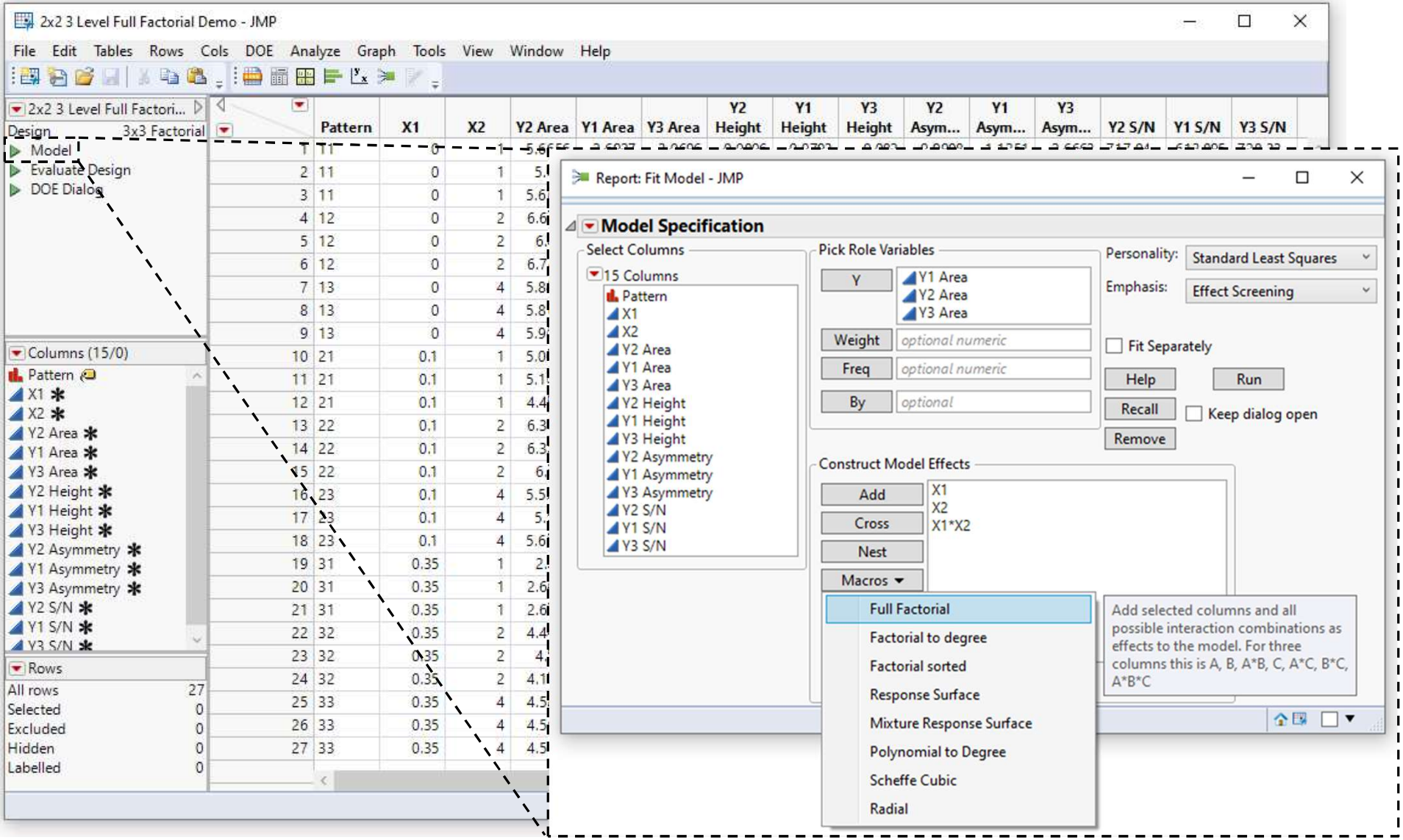
Response Surface:
Axial Points, Run Order, Replicates

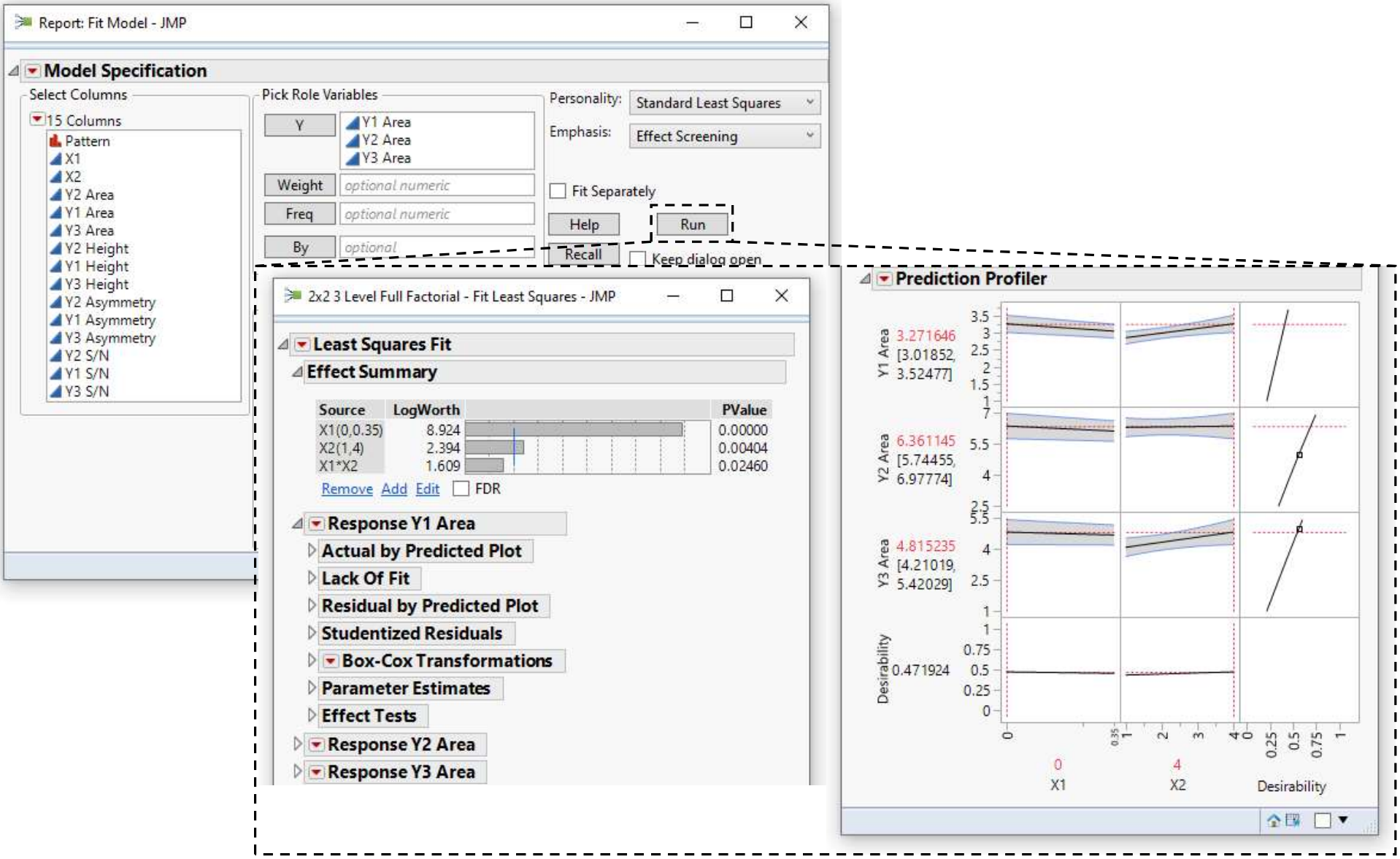
2 Factor

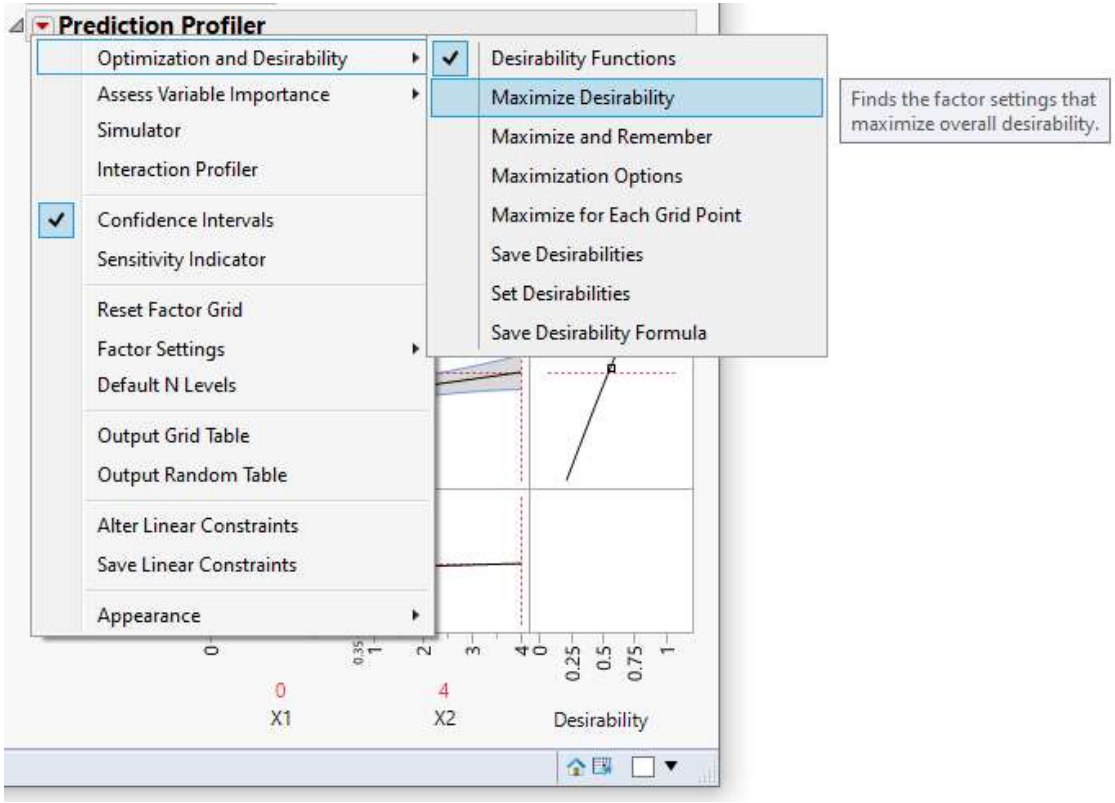


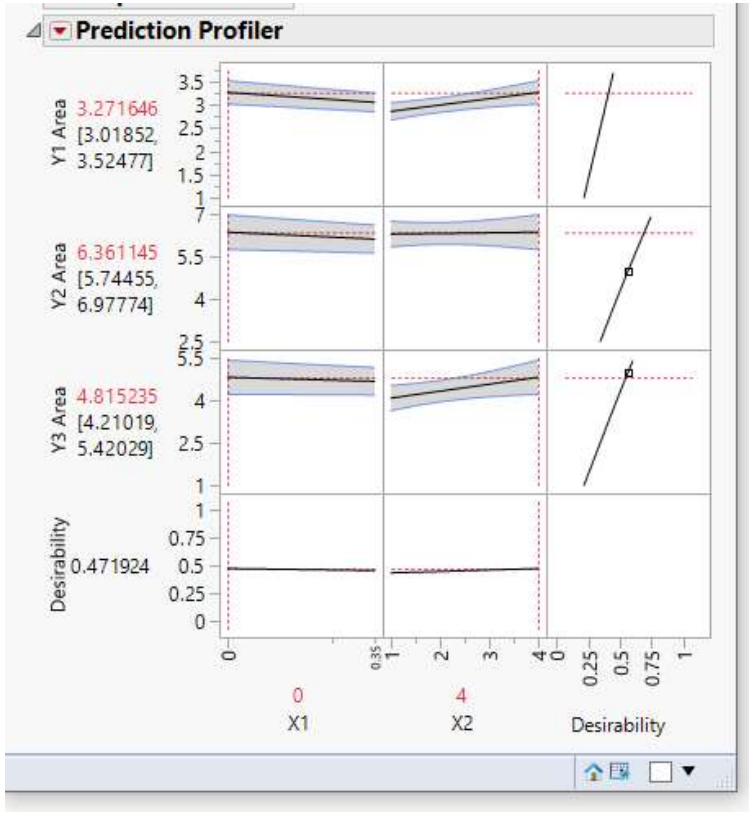
3 Factor




2x2 3 Level Full Factorial Demo - JMP
File Edit Tables Rows Cols DOE Analyze Graph Tools View Window Help
2x2 3 Level Full Factori...
Design 3x3 Factorial
Model
Evaluate Design
DOE Dialog
Columns (15/0)
Pattern
X1
X2
Y2 Area
Y1 Area
Y3 Area
Y2 Height
Y1 Height
Y3 Height
Y2 Asymmetry
Y1 Asymmetry
Y3 Asymmetry
Y2 S/N
Y1 S/N
Y3 S/N
Rows
All rows 27
Selected 0
Excluded 0
Hidden 0
Labelled 0
Pattern X1 X2 Y2 Area Y1 Area Y3 Area Y2 Height Y1 Height Y3 Height Y2 Asym... Y1 Asym... Y3 Asym... Y2 S/N Y1 S/N Y3 S/N
1 11 0 1
2 11 0 1 5.
3 11 0 1 5.6
4 12 0 2 6.6
5 12 0 2 6.
6 12 0 2 6.7
7 13 0 4 5.8
8 13 0 4 5.8
9 13 0 4 5.9
10 21 0.1 1 5.0
11 21 0.1 1 5.1
12 21 0.1 1 4.4
13 22 0.1 2 6.3
14 22 0.1 2 6.3
15 22 0.1 2 6.
16 23 0.1 4 5.5
17 23 0.1 4 5.
18 23 0.1 4 5.6
19 31 0.35 1 2.
20 31 0.35 1 2.6
21 31 0.35 1 2.6
22 32 0.35 2 4.4
23 32 0.35 2 4.
24 32 0.35 2 4.1
25 33 0.35 4 4.5
26 33 0.35 4 4.5
27 33 0.35 4 4.5
Report: Fit Model - JMP
Model Specification
Select Columns
15 Columns
Pattern
X1
X2
Y2 Area
Y1 Area
Y3 Area
Y2 Height
Y1 Height
Y3 Height
Y2 Asymmetry
Y1 Asymmetry
Y3 Asymmetry
Y2 S/N
Y1 S/N
Y3 S/N
Pick Role Variables
Y
Y1 Area
Y2 Area
Y3 Area
Weight optional numeric
Freq optional numeric
By optional
Personality: Standard Least Squares
Emphasis: Effect Screening
Fit Separately
Help
Run
Recall
Keep dialog open
Remove
Construct Model Effects
Add
Cross
Nest
Macros
X1
X2
X1*X2
Full Factorial
Factorial to degree
Factorial sorted
Response Surface
Mixture Response Surface
Polynomial to Degree
Scheffe Cubic
Radial
Add selected columns and all possible interaction combinations as effects to the model. For three columns this is A, B, A*B, C, A*C, B*C, A*B*C


Report: Fit Model - JMP
Model Specification
Select Columns
15 Columns
Pattern
X1
X2
Y2 Area
Y1 Area
Y3 Area
Y2 Height
Y1 Height
Y3 Height
Y2 Asymmetry
Y1 Asymmetry
Y3 Asymmetry
Y2 S/N
Y1 S/N
Y3 S/N
Pick Role Variables
Y
Y1 Area
Y2 Area
Y3 Area
Weight
optional numeric
Freq
optional numeric
By
optional
Personality:
Standard Least Squares
Emphasis:
Effect Screening
Fit Separately
Help
Run
Recall
Keep dialog open
2x2 3 Level Full Factorial - Fit Least Squares - JMP
Least Squares Fit
Effect Summary
Source
LogWorth
PValue
X1(0,0.35)
8.924
0.00000
X2(1,4)
2.394
0.00404
X1*X2
1.609
0.02460
Remove
Add
Edit
FDR
Response Y1 Area
Actual by Predicted Plot
Lack Of Fit
Residual by Predicted Plot
Studentized Residuals
Box-Cox Transformations
Parameter Estimates
Effect Tests
Response Y2 Area
Response Y3 Area
Prediction Profiler
Y1 Area
3.271646
[3.01852, 3.52477]
Y2 Area
6.361145
[5.74455, 6.97774]
Y3 Area
4.815235
[4.21019, 5.42029]
Desirability
0.471924
0
4
X1
X2
Desirability

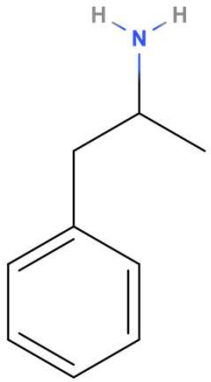

Prediction Profiler
Optimization and Desirability
Assess Variable Importance
Simulator
Interaction Profiler
Confidence Intervals
Sensitivity Indicator
Reset Factor Grid
Factor Settings
Default N Levels
Output Grid Table
Output Random Table
Alter Linear Constraints
Save Linear Constraints
Appearance
Desirability Functions
Maximize Desirability
Maximize and Remember
Maximization Options
Maximize for Each Grid Point
Save Desirabilities
Set Desirabilities
Save Desirability Formula
Finds the factor settings that maximize overall desirability.
0
4
X1
X2
Desirability


Prediction Profiler
Y1 Area
3.271646
[3.01852, 3.52477]
Y2 Area
6.361145
[5.74455, 6.97774]
Y3 Area
4.815235
[4.21019, 5.42029]
Desirability
0.471924
0
4
X1
X2
Desirability

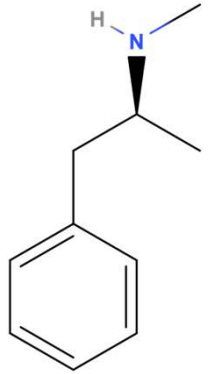
Dimension Reduction, Data Analysis, and Method Comparison

Principal Components Analysis and Discriminate Analysis

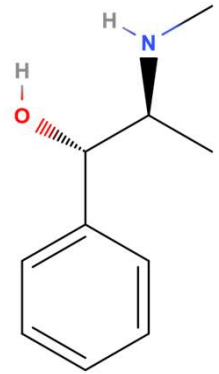
Molecule Differentiation with VUV



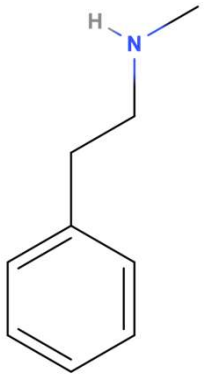
Amphetamine



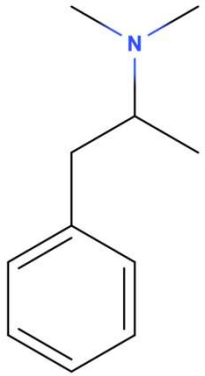
Methamphetamine



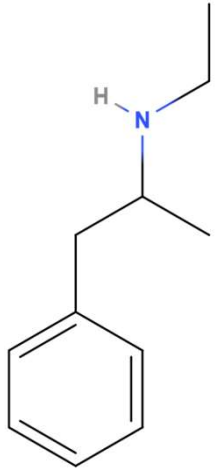
Pseudoephedrine



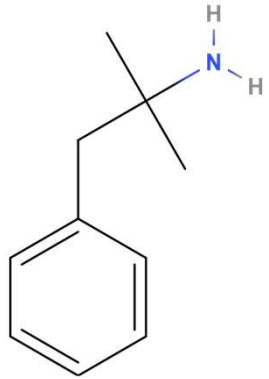
Methylphenethylamine



Dimethylamphetamine



Ethylamphetamine



Phentermine

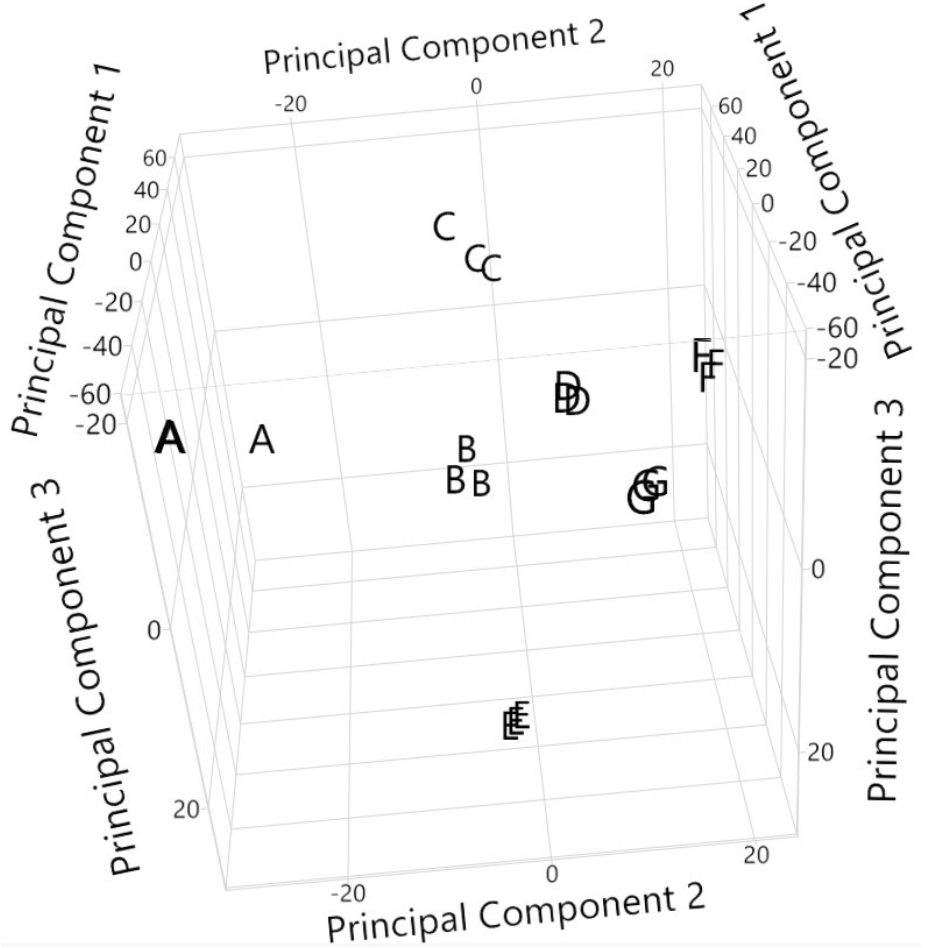
Squared Euclidian Distance Tables

	Pseudoephedrine (A)	Amphetamine (B)	Methylphenethylamine (C)	Methamphetamine (D)	Phentermine (E)	Dimethylamphetamine (F)	Ethylamphetamine (G)	Squared Euclidian Distance (SED)
	0.0377	1.3324	1.8717	1.0488	1.1414	1.1167	1.0869	Pseudoephedrine (A)
Pseudoephedrine (A)	0.9997		0.1000	0.5405	0.2650	0.3978	0.9721	0.8669	Amphetamine (B)
Amphetamine (B)	0.9944	0.9992		0.1329	0.6764	2.9698	1.4793	1.8467	Methylphenethylamine (C)
Methylphenethylamine (C)	0.9933	0.9960	0.9989		0.0650	1.1701	0.4607	0.4349	Methamphetamine (D)
Methamphetamine (D)	0.9947	0.9979	0.9960	0.9995		0.0256	1.2290	0.5798	Phentermine (E)
Phentermine (E)	0.9916	0.9945	0.9865	0.9949	0.9998		0.0330	0.3414	Dimethylamphetamine (F)
Dimethylamphetamine (F)	0.9932	0.9942	0.9927	0.9975	0.9924	0.9997		0.0282	Ethylamphetamine (G)
Ethylamphetamine (G)	0.9923	0.9951	0.9902	0.9977	0.9966	0.9976	0.9998	
Correlation Coefficient (r)	Pseudoephedrine (A)	Amphetamine (B)	Methylphenethylamine (C)	Methamphetamine (D)	Phentermine (E)	Dimethylamphetamine (F)	Ethylamphetamine (G)	

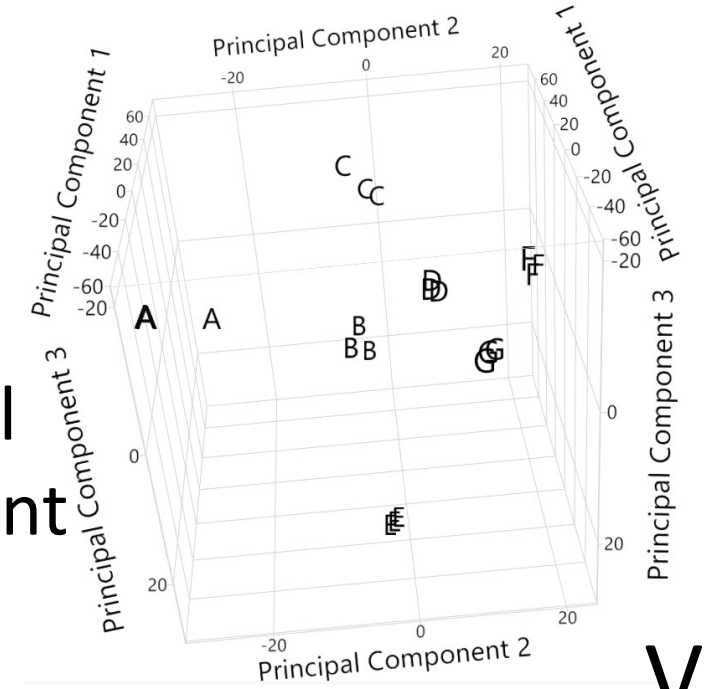
Correlation Coefficient Tables

VS

Principal Component Plots



Principal Component Plots



VS

		Predicted						
	Class	**A**	**B**	**C**	**D**	**E**	**F**	**G**
Actual	**A**	3	0	0	0	0	0	0
	B	0	3	0	0	0	0	0
	C	0	0	3	0	0	0	0
	D	0	0	0	3	0	0	0
	E	0	0	0	0	3	0	0
	F	0	0	0	0	0	3	0
	G	0	0	0	0	0	0	3

Linear Discriminate Analysis Score Summaries

Source	Count	Number Misclassified	Percent Misclassified	Entropy RSquare	-2LogLikelihood
Training	21	0	0	1	0

Linear Discriminate Analysis Scores

Row	Actual	SqDist(Actual)	Prob(Actual)	-Log(Prob)	Predicted	Prob(Pred)
1	Pseudoephedrine	2.867419075	1.0000	0.000	Pseudoephedrine	1.0000
2	Pseudoephedrine	4.756218574	1.0000	0.000	Pseudoephedrine	1.0000
3	Pseudoephedrine	0.85105816	1.0000	0.000	Pseudoephedrine	1.0000
4	Amphetamine	1.339068078	1.0000	0.000	Amphetamine	1.0000
5	Amphetamine	5.049067188	1.0000	0.000	Amphetamine	1.0000
6	Amphetamine	2.613566645	1.0000	0.000	Amphetamine	1.0000
7	Methylphenethylamine	0.559130435	1.0000	0.000	Methylphenethylamine	1.0000
8	Methylphenethylamine	2.21665668	1.0000	0.000	Methylphenethylamine	1.0000
9	Methylphenethylamine	4.661519032	1.0000	0.000	Methylphenethylamine	1.0000
10	Methamphetamine	0.39101123	1.0000	0.000	Methamphetamine	1.0000
11	Methamphetamine	0.798695716	1.0000	0.000	Methamphetamine	1.0000
12	Methamphetamine	0.271173389	1.0000	0.000	Methamphetamine	1.0000
13	Phentermine	0.054093181	1.0000	0.000	Phentermine	1.0000
14	Phentermine	0.182454685	1.0000	0.000	Phentermine	1.0000
15	Phentermine	0.146205638	1.0000	0.000	Phentermine	1.0000
16	Dimethylamphetamine	5.340529115	1.0000	0.000	Dimethylamphetamine	1.0000
17	Dimethylamphetamine	3.477602163	1.0000	0.000	Dimethylamphetamine	1.0000
18	Dimethylamphetamine	2.338286102	1.0000	0.000	Dimethylamphetamine	1.0000
19	Ethylamphetamine	2.357417628	1.0000	0.000	Ethylamphetamine	1.0000
20	Ethylamphetamine	1.577573617	1.0000	0.000	Ethylamphetamine	1.0000
21	Ethylamphetamine	0.151253667	1.0000	0.000	Ethylamphetamine	1.0000

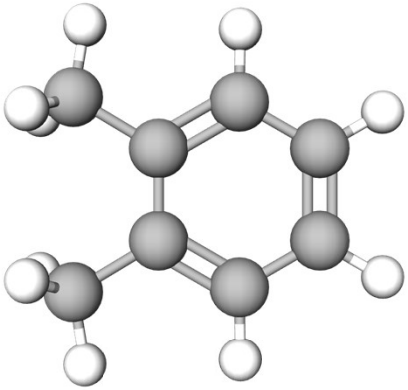
VS

Linear Discriminate Analysis Score Summaries

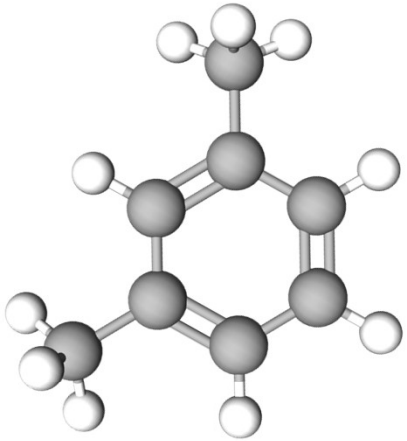
		Predicted						
	Class	A	B	C	D	E	F	G
Actual	A	3	0	0	0	0	0	0
	B	0	3	0	0	0	0	0
	C	0	0	3	0	0	0	0
	D	0	0	0	3	0	0	0
	E	0	0	0	0	3	0	0
	F	0	0	0	0	0	3	0
	G	0	0	0	0	0	0	3

Source	Count	Number Misclassified	Percent Misclassified	Entropy RSquare	-2LogLikelihood
Training	21	0	0	1	0

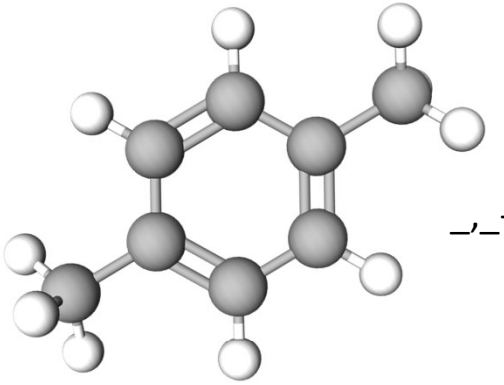
Method Comparison



1,2

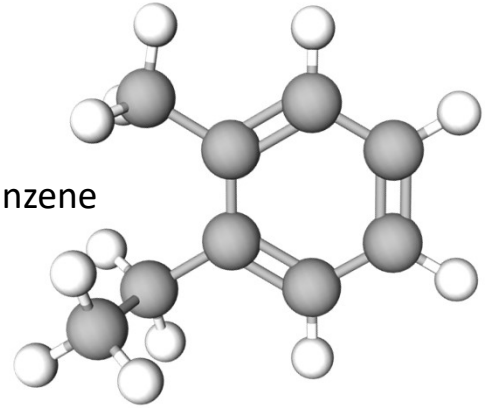


1,3

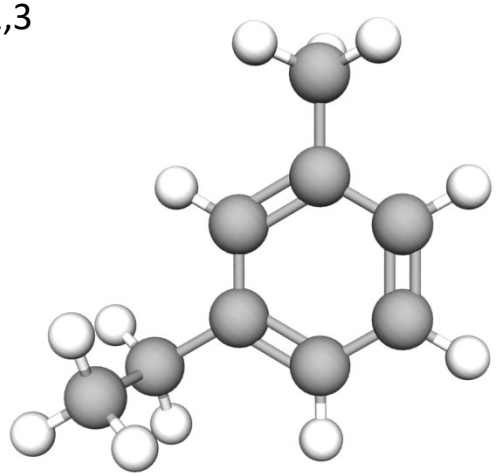


_,_-Dimethylbenzene

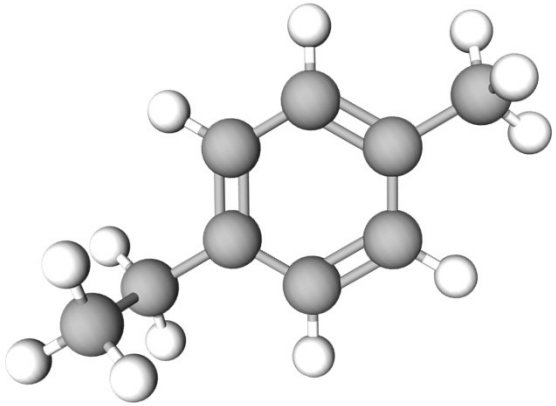
-Ethyl--Methylbenzene



1-2



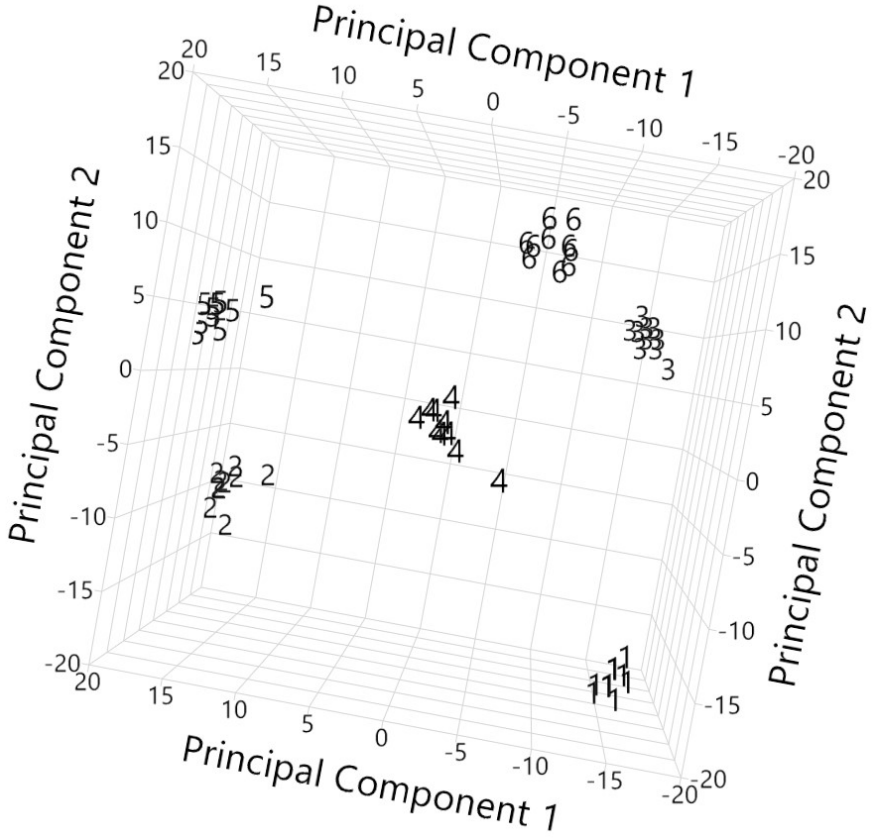
1-3



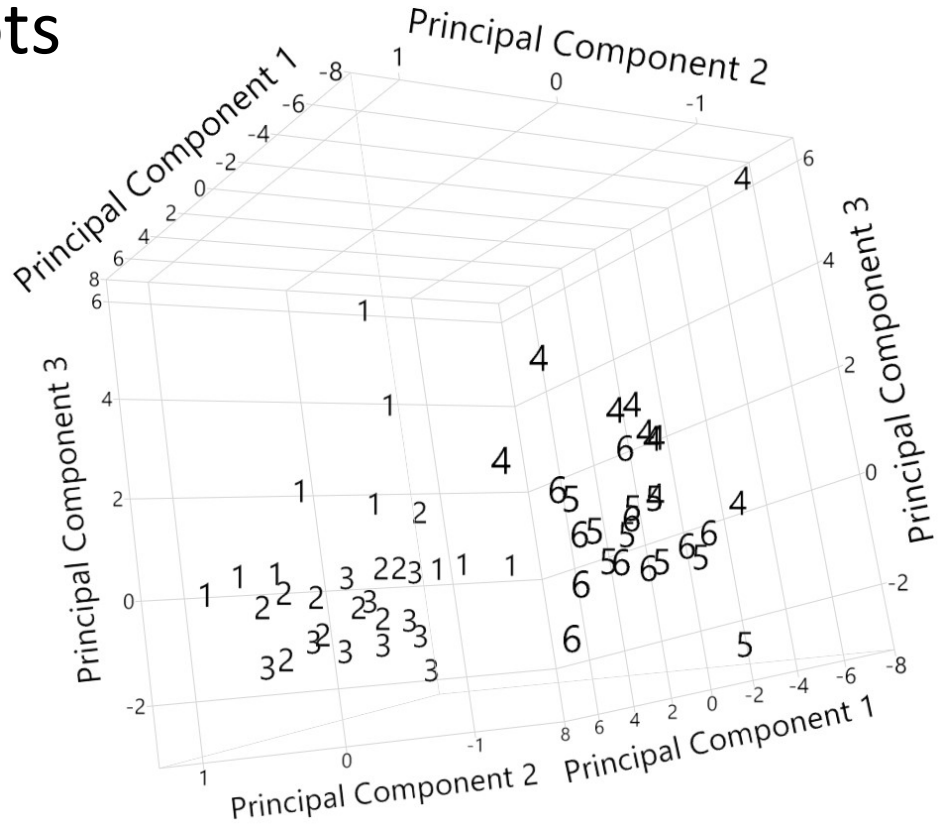
1-4

Principal Component Plots

VUV



MS



Linear Discriminate Analysis Scores

VUV

Row	Actual	SqDist(Actual)	Prob(Actual)	-Log(Prob)	Predicted	Prob(Pred)	Others
1	1-Ethyl-4-methylbenzene	2.37601	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
2	1-Ethyl-4-methylbenzene	3.06437	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
3	1-Ethyl-4-methylbenzene	2.73289	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
4	1-Ethyl-4-methylbenzene	3.55330	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
5	1-Ethyl-4-methylbenzene	1.82715	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
6	1-Ethyl-4-methylbenzene	4.10262	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
7	1-Ethyl-4-methylbenzene	5.03929	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
8	1-Ethyl-4-methylbenzene	2.53623	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
9	1-Ethyl-4-methylbenzene	2.31056	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
10	1-Ethyl-4-methylbenzene	4.45136	1.0000	0.000	1-Ethyl-4-methylbenzene	1.0000	
11	1-Ethyl-3-methylbenzene	2.80594	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
12	1-Ethyl-3-methylbenzene	2.91344	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
13	1-Ethyl-3-methylbenzene	1.48842	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
14	1-Ethyl-3-methylbenzene	1.88168	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
15	1-Ethyl-3-methylbenzene	0.27451	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
16	1-Ethyl-3-methylbenzene	1.03543	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
17	1-Ethyl-3-methylbenzene	6.29358	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
18	1-Ethyl-3-methylbenzene	1.38884	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
19	1-Ethyl-3-methylbenzene	1.22881	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
20	1-Ethyl-3-methylbenzene	9.81248	1.0000	0.000	1-Ethyl-3-methylbenzene	1.0000	
21	1-Ethyl-2-methylbenzene	4.78729	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
22	1-Ethyl-2-methylbenzene	0.26713	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
23	1-Ethyl-2-methylbenzene	2.59148	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
24	1-Ethyl-2-methylbenzene	1.47437	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
25	1-Ethyl-2-methylbenzene	16.11941	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
26	1-Ethyl-2-methylbenzene	2.05877	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
27	1-Ethyl-2-methylbenzene	0.23978	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
28	1-Ethyl-2-methylbenzene	3.22295	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
29	1-Ethyl-2-methylbenzene	6.97902	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
30	1-Ethyl-2-methylbenzene	2.37624	1.0000	0.000	1-Ethyl-2-methylbenzene	1.0000	
31	1,4-Dimethylbenzene	0.65749	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
32	1,4-Dimethylbenzene	1.56110	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
33	1,4-Dimethylbenzene	5.44942	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
34	1,4-Dimethylbenzene	0.99260	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
35	1,4-Dimethylbenzene	2.85628	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
36	1,4-Dimethylbenzene	0.38890	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
37	1,4-Dimethylbenzene	0.68730	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
38	1,4-Dimethylbenzene	3.60755	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
39	1,4-Dimethylbenzene	2.10686	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
40	1,4-Dimethylbenzene	1.00198	1.0000	0.000	1,4-Dimethylbenzene	1.0000	
41	1,3-Dimethylbenzene	1.15920	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
42	1,3-Dimethylbenzene	0.41693	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
43	1,3-Dimethylbenzene	2.16777	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
44	1,3-Dimethylbenzene	1.70524	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
45	1,3-Dimethylbenzene	8.50800	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
46	1,3-Dimethylbenzene	1.22893	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
47	1,3-Dimethylbenzene	0.97001	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
48	1,3-Dimethylbenzene	6.42828	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
49	1,3-Dimethylbenzene	3.90486	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
50	1,3-Dimethylbenzene	0.40507	1.0000	0.000	1,3-Dimethylbenzene	1.0000	
51	1,2-Dimethylbenzene	0.64059	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
52	1,2-Dimethylbenzene	0.52348	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
53	1,2-Dimethylbenzene	2.52986	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
54	1,2-Dimethylbenzene	0.54832	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
55	1,2-Dimethylbenzene	2.82588	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
56	1,2-Dimethylbenzene	1.60093	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
57	1,2-Dimethylbenzene	0.75215	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
58	1,2-Dimethylbenzene	0.78858	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
59	1,2-Dimethylbenzene	2.09435	1.0000	0.000	1,2-Dimethylbenzene	1.0000	
60	1,2-Dimethylbenzene	2.25870	1.0000	0.000	1,2-Dimethylbenzene	1.0000	

MS

Row	Actual	SqDist(Actual)	Prob(Actual)	-Log(Prob)		Predicted	Prob(Pred)	Others
1	1-Ethyl-4-methylbenzene	0.42406	0.5175	0.659		1-Ethyl-4-methylbenzene	0.5175	1-Ethyl-3-methylbenzene 0.45
2	1-Ethyl-4-methylbenzene	0.64191	0.6218	0.475		1-Ethyl-4-methylbenzene	0.6218	1-Ethyl-2-methylbenzene 0.17 1-Ethyl-3-methylbenzene 0.20
3	1-Ethyl-4-methylbenzene	2.36280	0.3265	1.119	*	1-Ethyl-3-methylbenzene	0.6352	
4	1-Ethyl-4-methylbenzene	0.20536	0.6122	0.491		1-Ethyl-4-methylbenzene	0.6122	1-Ethyl-3-methylbenzene 0.32
5	1-Ethyl-4-methylbenzene	0.67108	0.4402	0.821	*	1-Ethyl-3-methylbenzene	0.4564	1-Ethyl-2-methylbenzene 0.10
6	1-Ethyl-4-methylbenzene	1.83933	0.7057	0.349		1-Ethyl-4-methylbenzene	0.7057	1-Ethyl-3-methylbenzene 0.23
7	1-Ethyl-4-methylbenzene	0.86245	0.4462	0.807		1-Ethyl-4-methylbenzene	0.4462	1-Ethyl-2-methylbenzene 0.32 1-Ethyl-3-methylbenzene 0.24
8	1-Ethyl-4-methylbenzene	1.66880	0.5757	0.552		1-Ethyl-4-methylbenzene	0.5757	1-Ethyl-3-methylbenzene 0.42
9	1-Ethyl-4-methylbenzene	0.29272	0.6297	0.463		1-Ethyl-4-methylbenzene	0.6297	1-Ethyl-2-methylbenzene 0.11 1-Ethyl-3-methylbenzene 0.26
10	1-Ethyl-4-methylbenzene	2.03802	0.2859	1.252	*	1-Ethyl-2-methylbenzene	0.4456	1-Ethyl-3-methylbenzene 0.27
11	1-Ethyl-3-methylbenzene	1.31235	0.3311	1.105	*	1-Ethyl-4-methylbenzene	0.6043	
12	1-Ethyl-3-methylbenzene	2.36802	0.2080	1.570	*	1-Ethyl-4-methylbenzene	0.4863	1-Ethyl-2-methylbenzene 0.31
13	1-Ethyl-3-methylbenzene	0.33468	0.4601	0.776		1-Ethyl-3-methylbenzene	0.4601	1-Ethyl-4-methylbenzene 0.46
14	1-Ethyl-3-methylbenzene	1.10959	0.6212	0.476		1-Ethyl-3-methylbenzene	0.6212	1-Ethyl-4-methylbenzene 0.36
15	1-Ethyl-3-methylbenzene	0.99246	0.4352	0.832	*	1-Ethyl-4-methylbenzene	0.5174	
16	1-Ethyl-3-methylbenzene	0.72664	0.4402	0.821		1-Ethyl-3-methylbenzene	0.4402	1-Ethyl-2-methylbenzene 0.13 1-Ethyl-4-methylbenzene 0.43
17	1-Ethyl-3-methylbenzene	2.77220	0.7030	0.352		1-Ethyl-3-methylbenzene	0.7030	1-Ethyl-4-methylbenzene 0.27
18	1-Ethyl-3-methylbenzene	45.30598	0.9891	0.011		1-Ethyl-3-methylbenzene	0.9891	
19	1-Ethyl-3-methylbenzene	3.40272	0.3952	0.928	*	1-Ethyl-4-methylbenzene	0.5988	
20	1-Ethyl-3-methylbenzene	0.55236	0.4419	0.817		1-Ethyl-3-methylbenzene	0.4419	1-Ethyl-2-methylbenzene 0.16 1-Ethyl-4-methylbenzene 0.40
21	1-Ethyl-2-methylbenzene	1.70890	0.2438	1.411	*	1-Ethyl-4-methylbenzene	0.4576	1-Ethyl-3-methylbenzene 0.30
22	1-Ethyl-2-methylbenzene	1.23800	0.5089	0.675		1-Ethyl-2-methylbenzene	0.5089	1-Ethyl-3-methylbenzene 0.16 1-Ethyl-4-methylbenzene 0.33
23	1-Ethyl-2-methylbenzene	2.92180	0.8915	0.115		1-Ethyl-2-methylbenzene	0.8915	
24	1-Ethyl-2-methylbenzene	0.42421	0.7133	0.338		1-Ethyl-2-methylbenzene	0.7133	1-Ethyl-4-methylbenzene 0.21
25	1-Ethyl-2-methylbenzene	0.57682	0.7473	0.291		1-Ethyl-2-methylbenzene	0.7473	1-Ethyl-3-methylbenzene 0.11 1-Ethyl-4-methylbenzene 0.14
26	1-Ethyl-2-methylbenzene	1.30832	0.5410	0.614		1-Ethyl-2-methylbenzene	0.5410	1-Ethyl-3-methylbenzene 0.23 1-Ethyl-4-methylbenzene 0.23
27	1-Ethyl-2-methylbenzene	0.64743	0.5723	0.558		1-Ethyl-2-methylbenzene	0.5723	1-Ethyl-3-methylbenzene 0.18 1-Ethyl-4-methylbenzene 0.24
28	1-Ethyl-2-methylbenzene	15.58065	0.9999	0.000		1-Ethyl-2-methylbenzene	0.9999	
29	1-Ethyl-2-methylbenzene	3.43099	0.1657	1.798	*	1-Ethyl-4-methylbenzene	0.4457	1-Ethyl-3-methylbenzene 0.39
30	1-Ethyl-2-methylbenzene	0.65558	0.9319	0.071		1-Ethyl-2-methylbenzene	0.9319	
31	1,4-Dimethylbenzene	1.00219	0.5747	0.554		1,4-Dimethylbenzene	0.5747	1,3-Dimethylbenzene 0.42
32	1,4-Dimethylbenzene	1.91160	0.7613	0.273		1,4-Dimethylbenzene	0.7613	1,3-Dimethylbenzene 0.24
33	1,4-Dimethylbenzene	0.29902	0.6547	0.424		1,4-Dimethylbenzene	0.6547	1,3-Dimethylbenzene 0.34
34	1,4-Dimethylbenzene	0.50908	0.4970	0.699		1,4-Dimethylbenzene	0.4970	1,3-Dimethylbenzene 0.49
35	1,4-Dimethylbenzene	6.26496	0.0577	2.853	*	1,2-Dimethylbenzene	0.7066	1,3-Dimethylbenzene 0.24
36	1,4-Dimethylbenzene	1.76126	0.4699	0.755	*	1,3-Dimethylbenzene	0.5142	
37	1,4-Dimethylbenzene	2.84770	0.7882	0.238		1,4-Dimethylbenzene	0.7882	1,3-Dimethylbenzene 0.21
38	1,4-Dimethylbenzene	1.20991	0.5494	0.599		1,4-Dimethylbenzene	0.5494	1,3-Dimethylbenzene 0.45
39	1,4-Dimethylbenzene	0.19845	0.5354	0.625		1,4-Dimethylbenzene	0.5354	1,3-Dimethylbenzene 0.46
40	1,4-Dimethylbenzene	0.32980	0.6305	0.461		1,4-Dimethylbenzene	0.6305	1,3-Dimethylbenzene 0.37
41	1,3-Dimethylbenzene	0.13131	0.5007	0.692		1,3-Dimethylbenzene	0.5007	1,4-Dimethylbenzene 0.49
42	1,3-Dimethylbenzene	1.71094	0.4129	0.884	*	1,4-Dimethylbenzene	0.5863	
43	1,3-Dimethylbenzene	0.57789	0.5354	0.625		1,3-Dimethylbenzene	0.5354	1,4-Dimethylbenzene 0.46
44	1,3-Dimethylbenzene	0.02806	0.5466	0.604		1,3-Dimethylbenzene	0.5466	1,4-Dimethylbenzene 0.44
45	1,3-Dimethylbenzene	0.71661	0.4188	0.870	*	1,4-Dimethylbenzene	0.5796	
46	1,3-Dimethylbenzene	3.34630	0.5487	0.600		1,3-Dimethylbenzene	0.5487	1,2-Dimethylbenzene 0.16 1,4-Dimethylbenzene 0.29
47	1,3-Dimethylbenzene	0.16595	0.5732	0.557		1,3-Dimethylbenzene	0.5732	1,4-Dimethylbenzene 0.40
48	1,3-Dimethylbenzene	1.75491	0.4538	0.790	*	1,4-Dimethylbenzene	0.5445	
49	1,3-Dimethylbenzene	6.37153	0.0412	3.189	*	1,2-Dimethylbenzene	0.9536	
50	1,3-Dimethylbenzene	0.55642	0.5434	0.610		1,3-Dimethylbenzene	0.5434	1,4-Dimethylbenzene 0.43
51	1,2-Dimethylbenzene	0.03193	0.9696	0.031		1,2-Dimethylbenzene	0.9696	
52	1,2-Dimethylbenzene	2.15029	0.9836	0.017		1,2-Dimethylbenzene	0.9836	
53	1,2-Dimethylbenzene	2.01796	0.4001	0.916	*	1,3-Dimethylbenzene	0.4494	1,4-Dimethylbenzene 0.15
54	1,2-Dimethylbenzene	4.34658	0.9978	0.002		1,2-Dimethylbenzene	0.9978	
55	1,2-Dimethylbenzene	0.31737	0.9476	0.054		1,2-Dimethylbenzene	0.9476	
56	1,2-Dimethylbenzene	1.29020	0.6623	0.412		1,2-Dimethylbenzene	0.6623	1,3-Dimethylbenzene 0.27
57	1,2-Dimethylbenzene	3.17236	0.2493	1.389	*	1,3-Dimethylbenzene	0.5464	1,4-Dimethylbenzene 0.20
58	1,2-Dimethylbenzene	13.62626	1.0000	0.000		1,2-Dimethylbenzene	1.0000	
59	1,2-Dimethylbenzene	3.42504	0.9953	0.005		1,2-Dimethylbenzene	0.9953	
60	1,2-Dimethylbenzene	1.55189	0.6638	0.410		1,2-Dimethylbenzene	0.6638	1,3-Dimethylbenzene 0.26

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