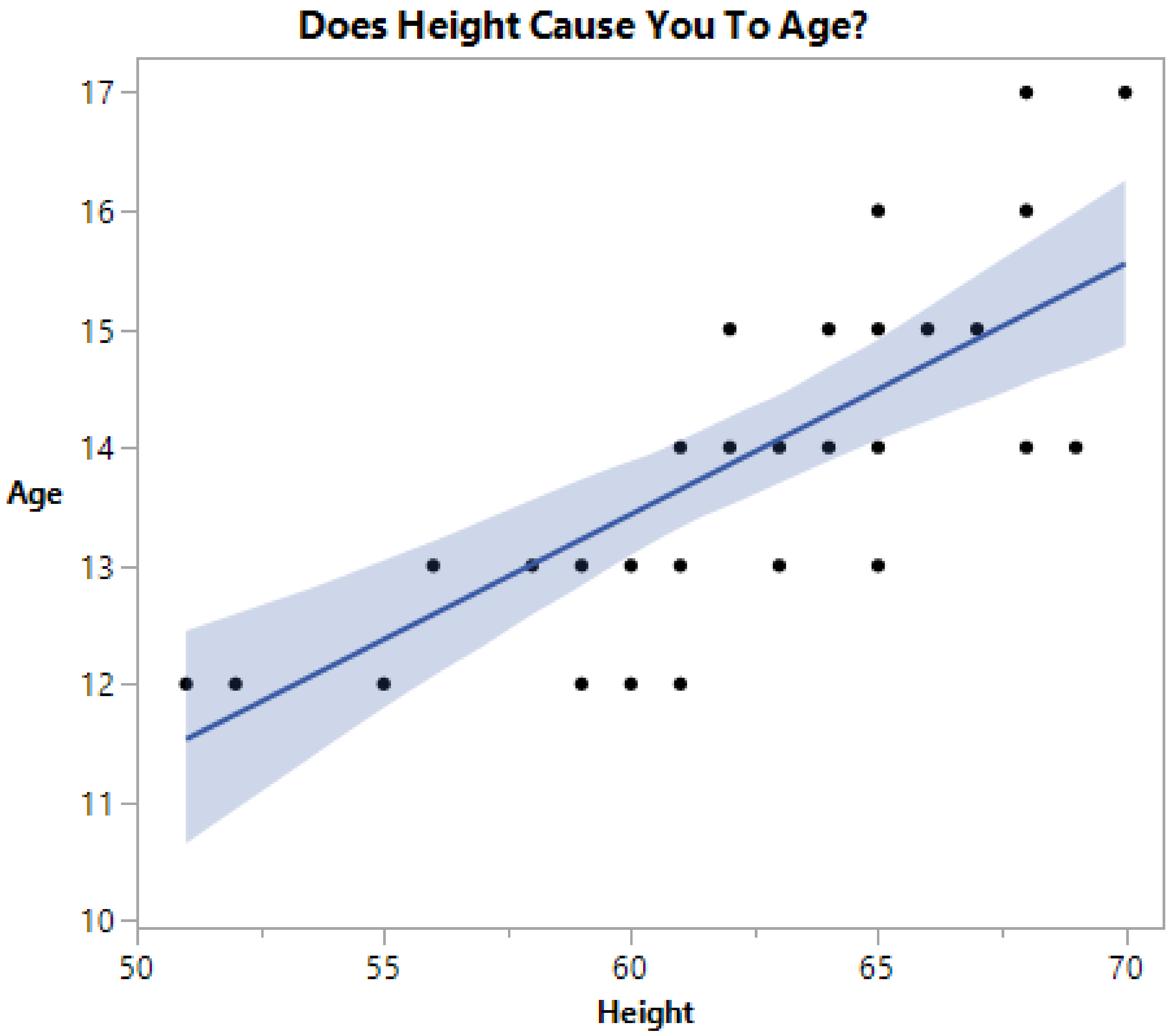
High Impact JMP Pro 19 Capabilities

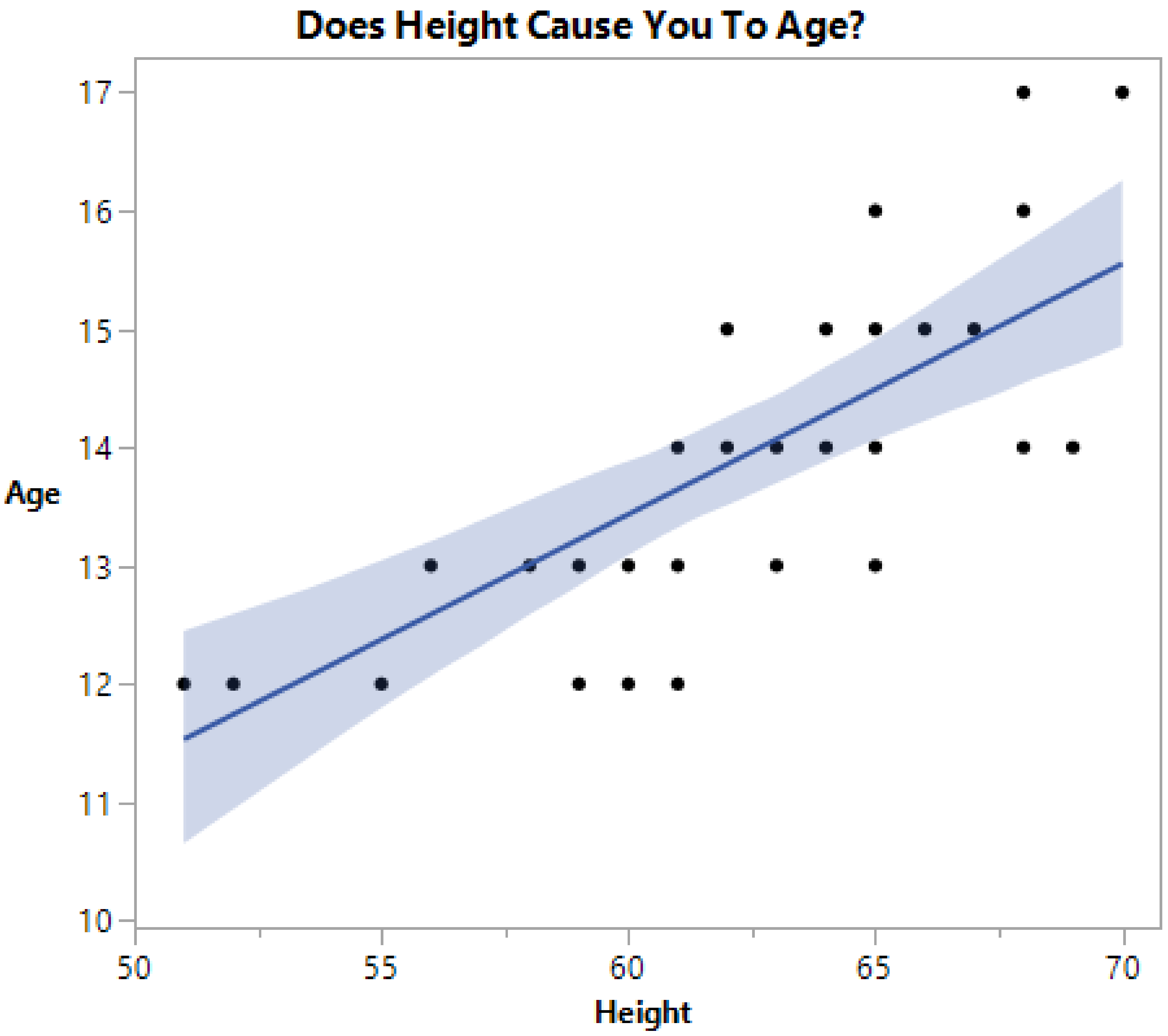
Chris Gotwalt

- **Causal Treatment**
- **Functional Data Explorer**
- **Bayesian Optimization**

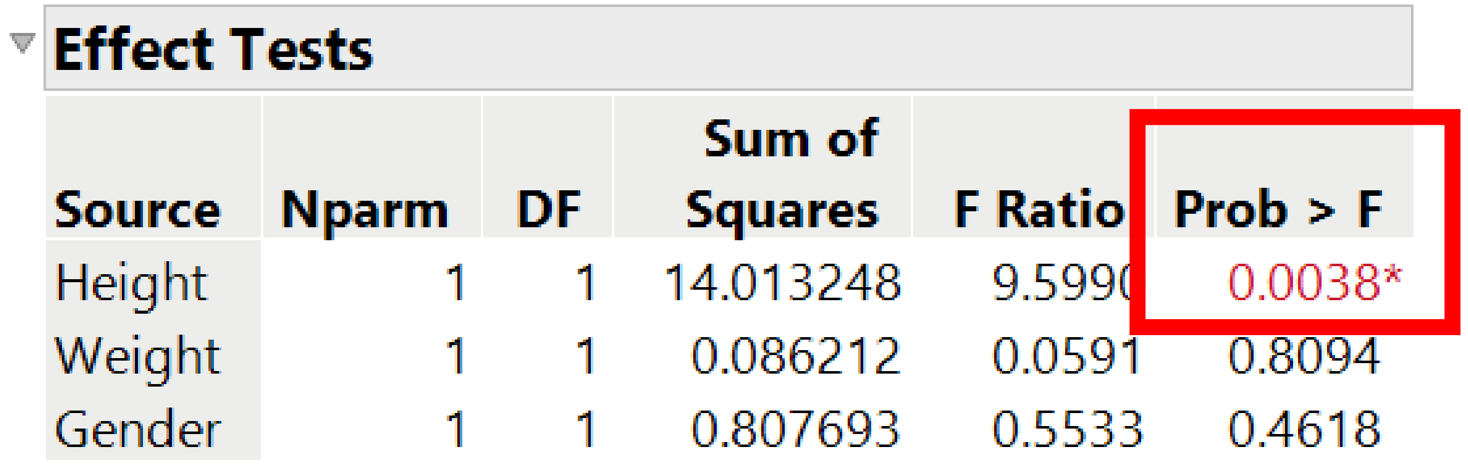
Causal Treatment



Causal Treatment



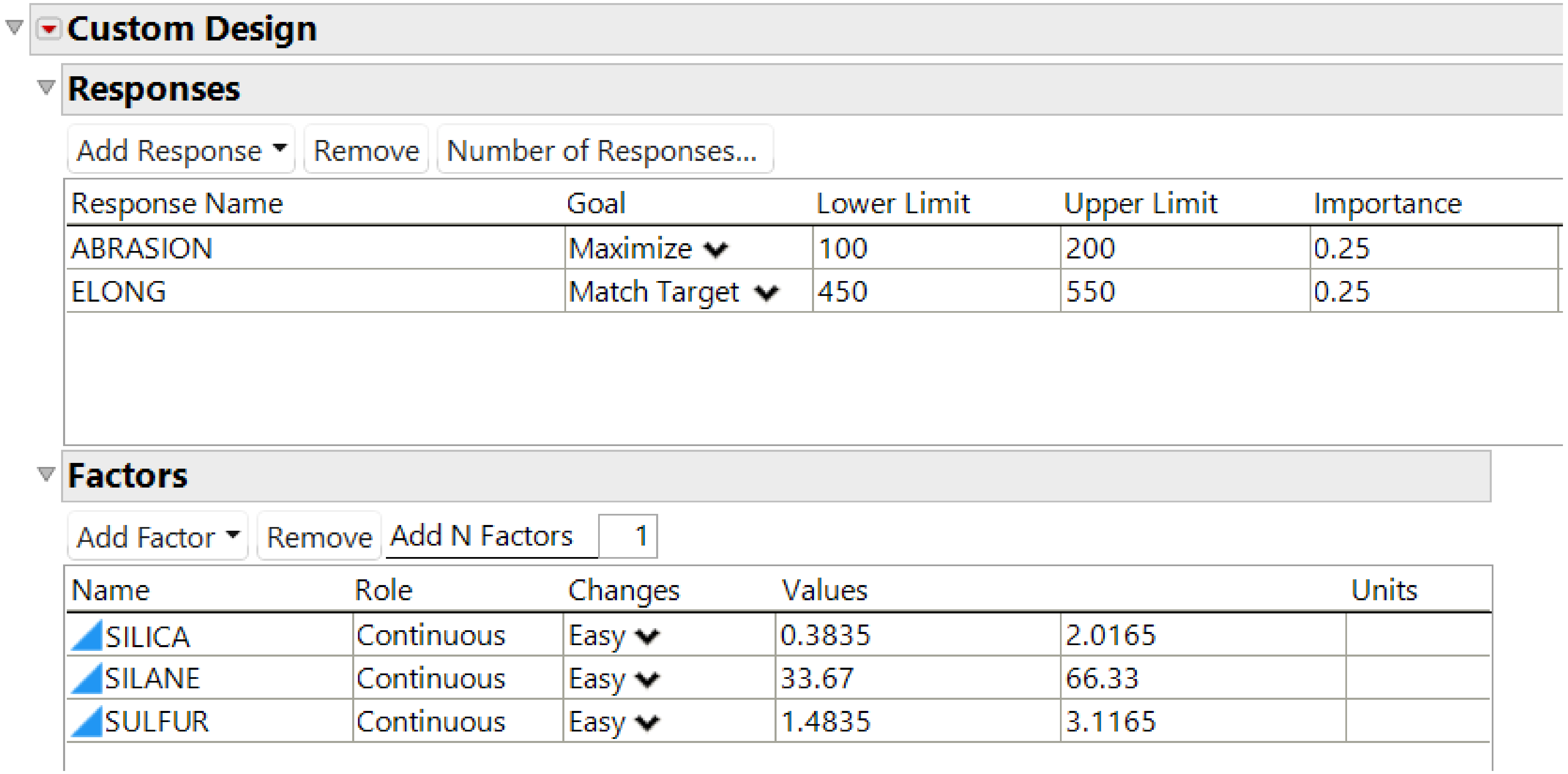
Does Height Cause You To Age?



Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
Height	1	1	14.013248	9.599	0.0038*
Weight	1	1	0.086212	0.0591	0.8094
Gender	1	1	0.807693	0.5533	0.4618

Causal Treatment



Custom Design

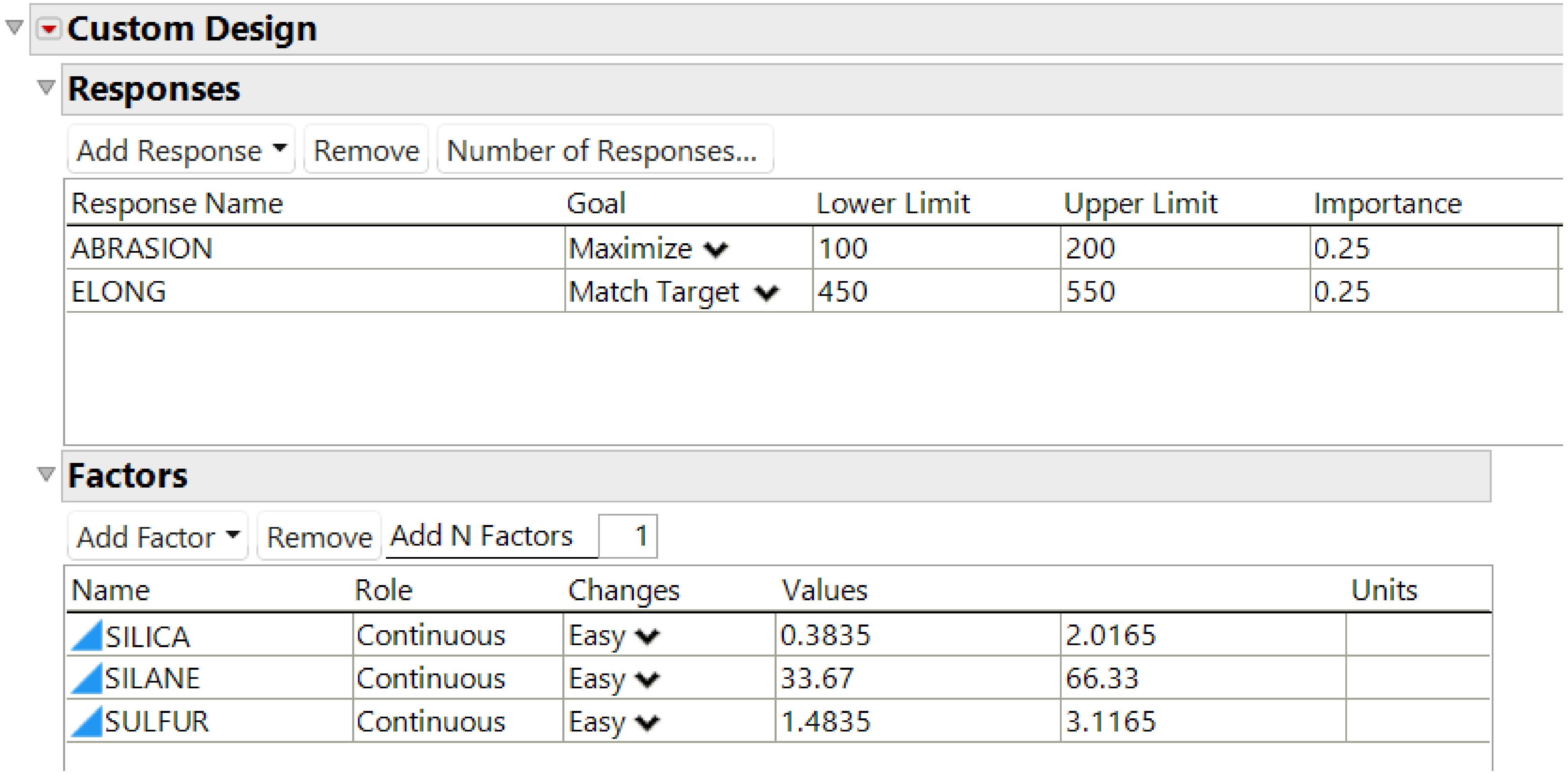
Responses

Response Name	Goal	Lower Limit	Upper Limit	Importance
ABRASION	Maximize	100	200	0.25
ELONG	Match Target	450	550	0.25

Factors

Name	Role	Changes	Values		Units
SILICA	Continuous	Easy	0.3835	2.0165	
SILANE	Continuous	Easy	33.67	66.33	
SULFUR	Continuous	Easy	1.4835	3.1165	

Causal Treatment



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"To find out what happens when you change something it is necessary to change it"
-George Box

Causal Treatment

Public Health

Water Pollutant $\xrightarrow{?}$ Birth Defects

Medicine

New Drug $\xrightarrow{?}$ Side Effect

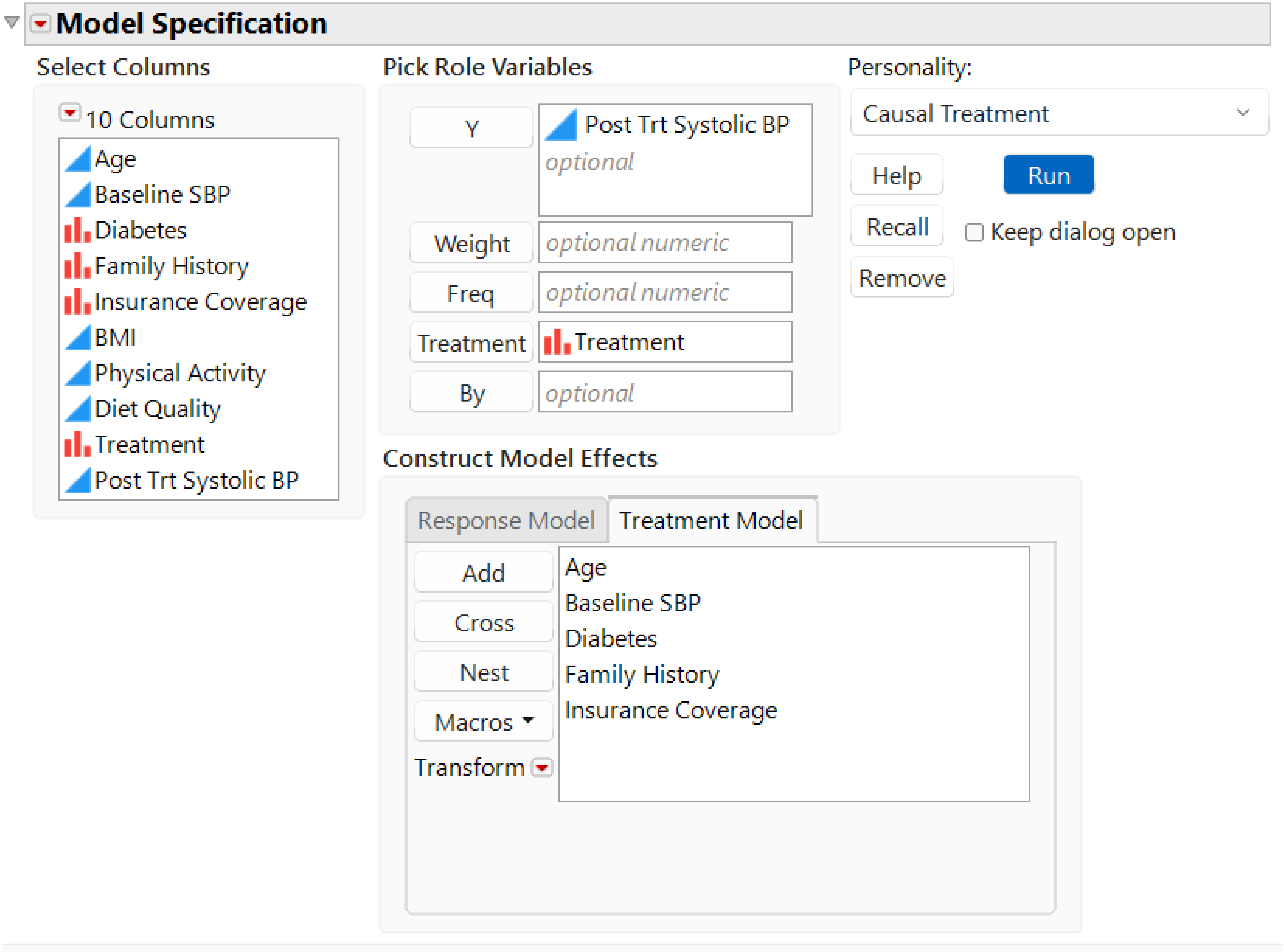
Policy

Education Program $\xrightarrow{?}$ Poverty Level

Marketing

Promotion $\xrightarrow{?}$ Purchase

Causal Treatment



Model Specification

Select Columns

10 Columns

- Age
- Baseline SBP
- Diabetes
- Family History
- Insurance Coverage
- BMI
- Physical Activity
- Diet Quality
- Treatment
- Post Trt Systolic BP

Pick Role Variables

Y: Post Trt Systolic BP

Weight: optional numeric

Freq: optional numeric

Treatment: Treatment

By: optional

Personality: Causal Treatment

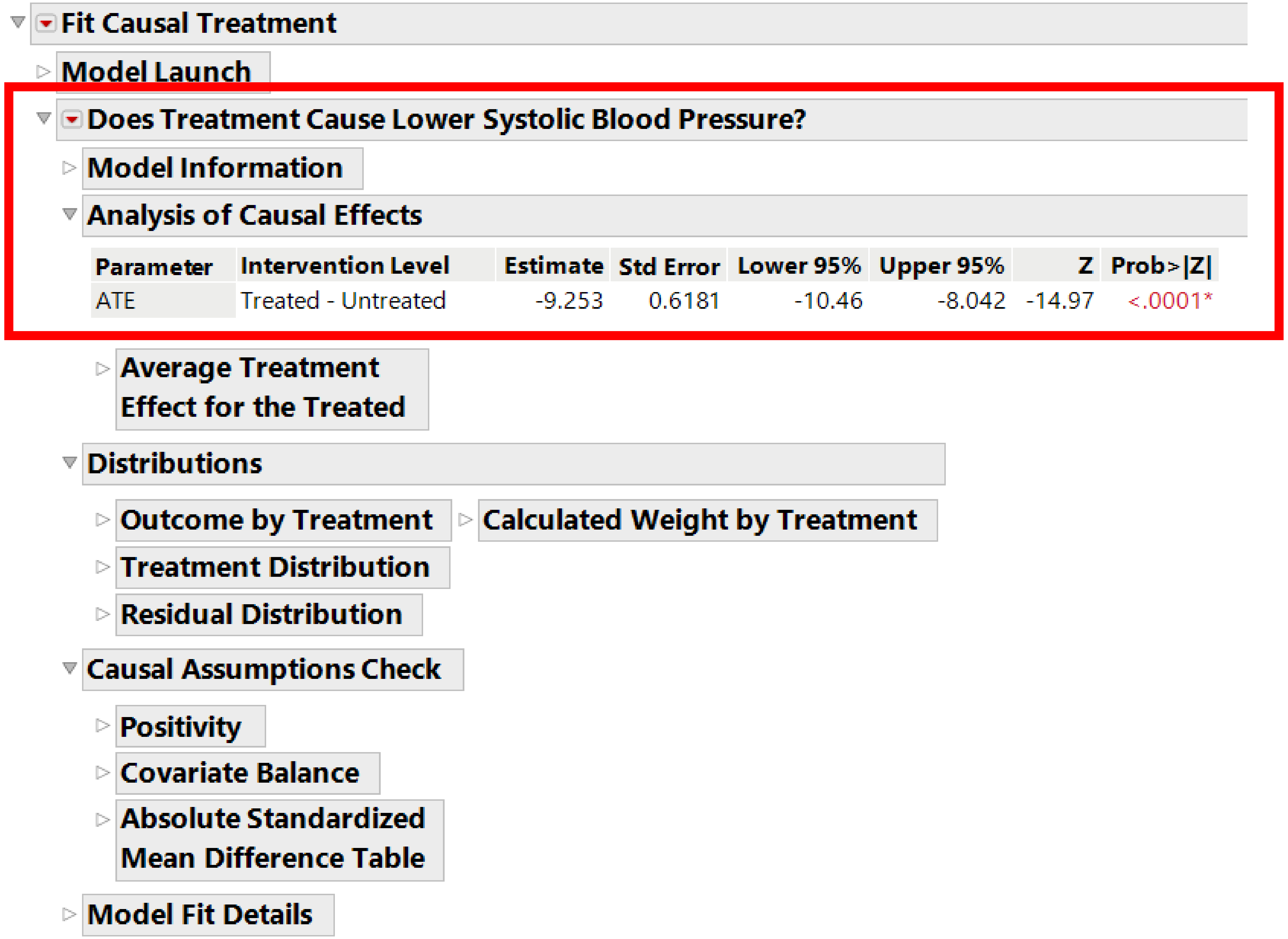
☐ Keep dialog open

Construct Model Effects

Treatment Model:

- Age
- Baseline SBP
- Diabetes
- Family History
- Insurance Coverage

Causal Treatment



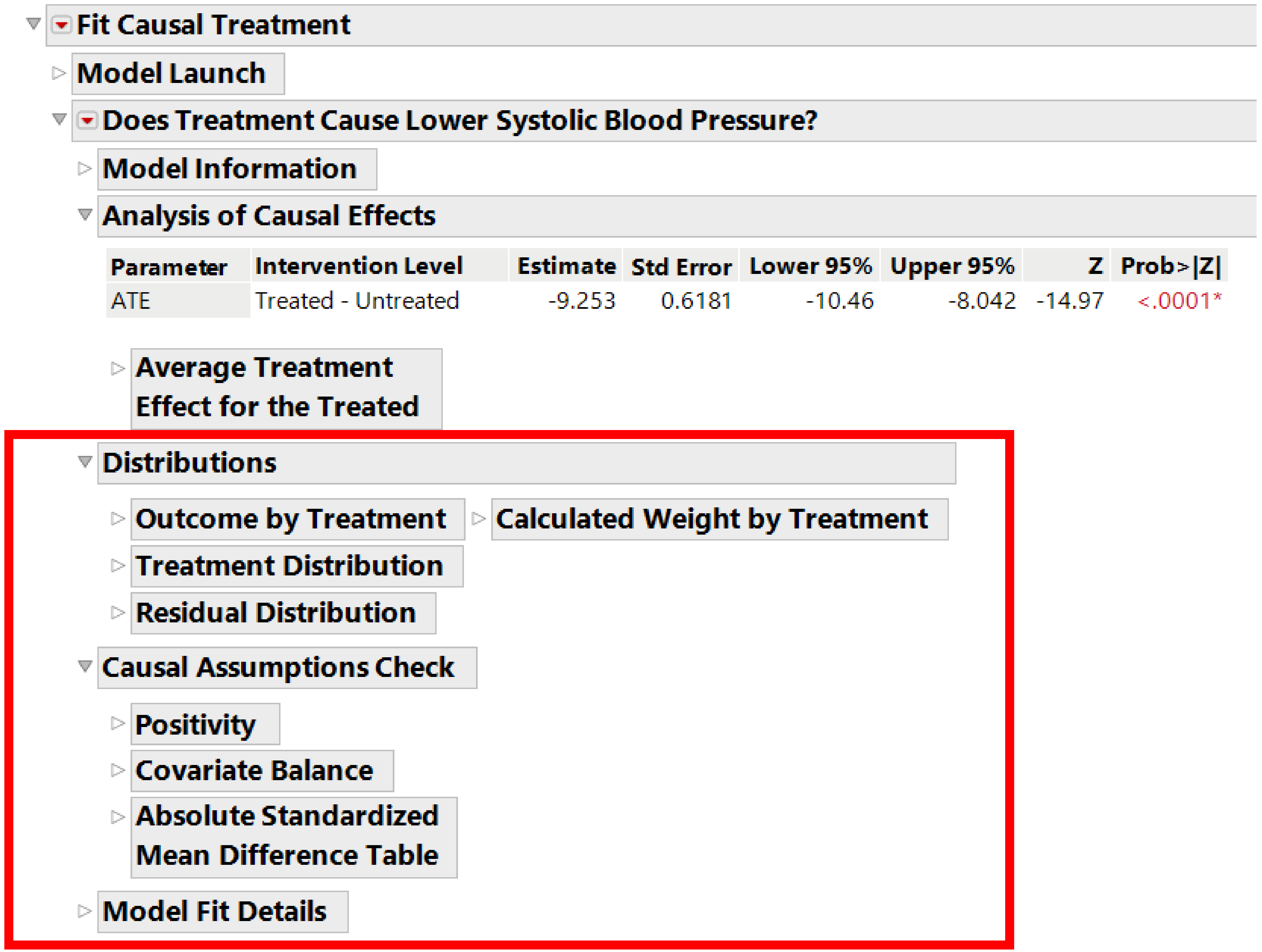
Fit Causal Treatment

- **Model Launch**
- **Does Treatment Cause Lower Systolic Blood Pressure?**
  - **Model Information**
  - **Analysis of Causal Effects**

Parameter	Intervention Level	Estimate	Std Error	Lower 95%	Upper 95%	Z	Prob>|Z|
ATE	Treated - Untreated	-9.253	0.6181	-10.46	-8.042	-14.97	<.0001*

  - **Average Treatment Effect for the Treated**
  - **Distributions**
    - **Outcome by Treatment**
    - **Calculated Weight by Treatment**
    - **Treatment Distribution**
    - **Residual Distribution**
  - **Causal Assumptions Check**
    - **Positivity**
    - **Covariate Balance**
    - **Absolute Standardized Mean Difference Table**
  - **Model Fit Details**

Causal Treatment



Fit Causal Treatment

Model Launch

Does Treatment Cause Lower Systolic Blood Pressure?

Model Information

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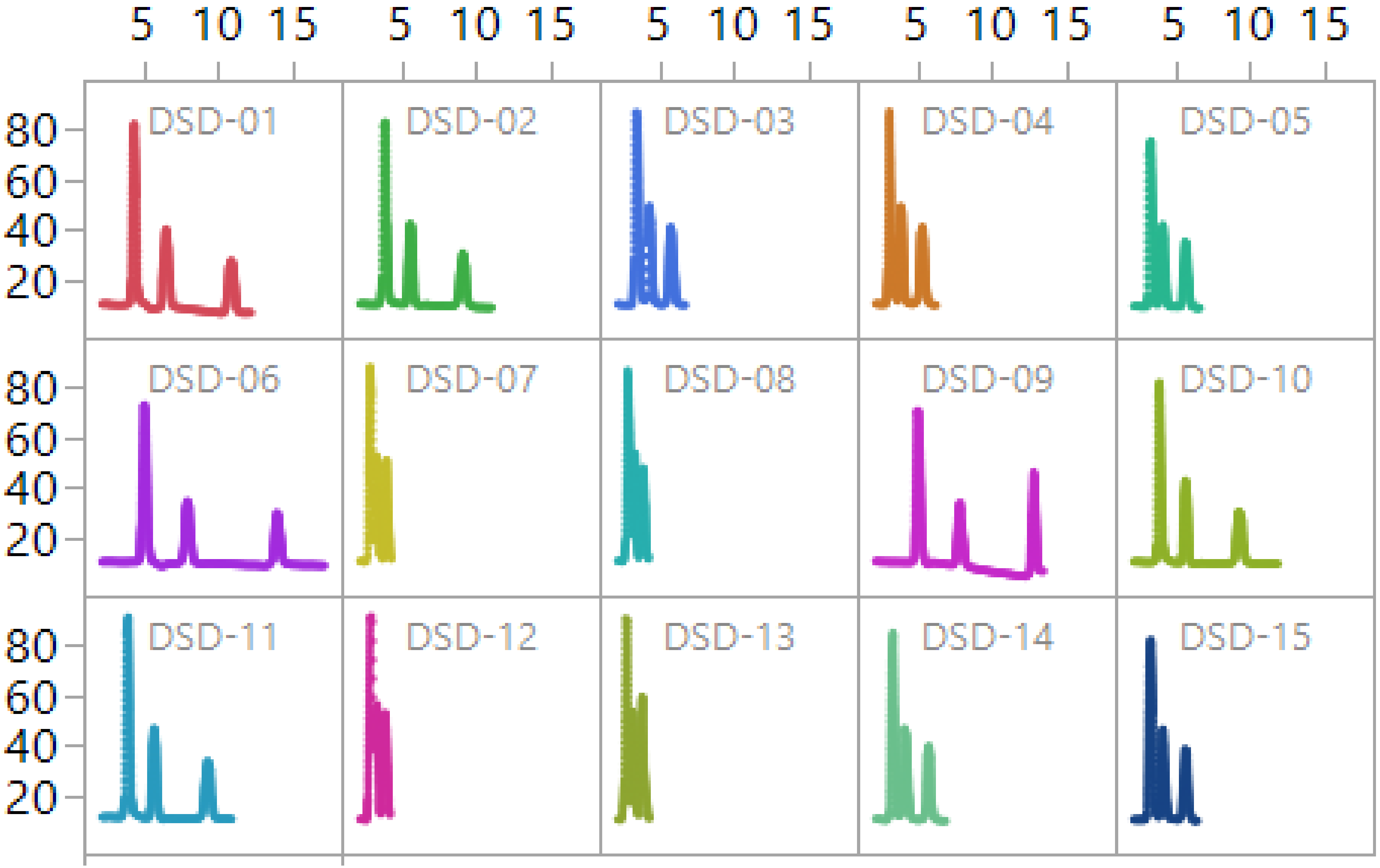
Model Fit Details

Functional Data Explorer

FDE Baseline Correction & Peak Modeling



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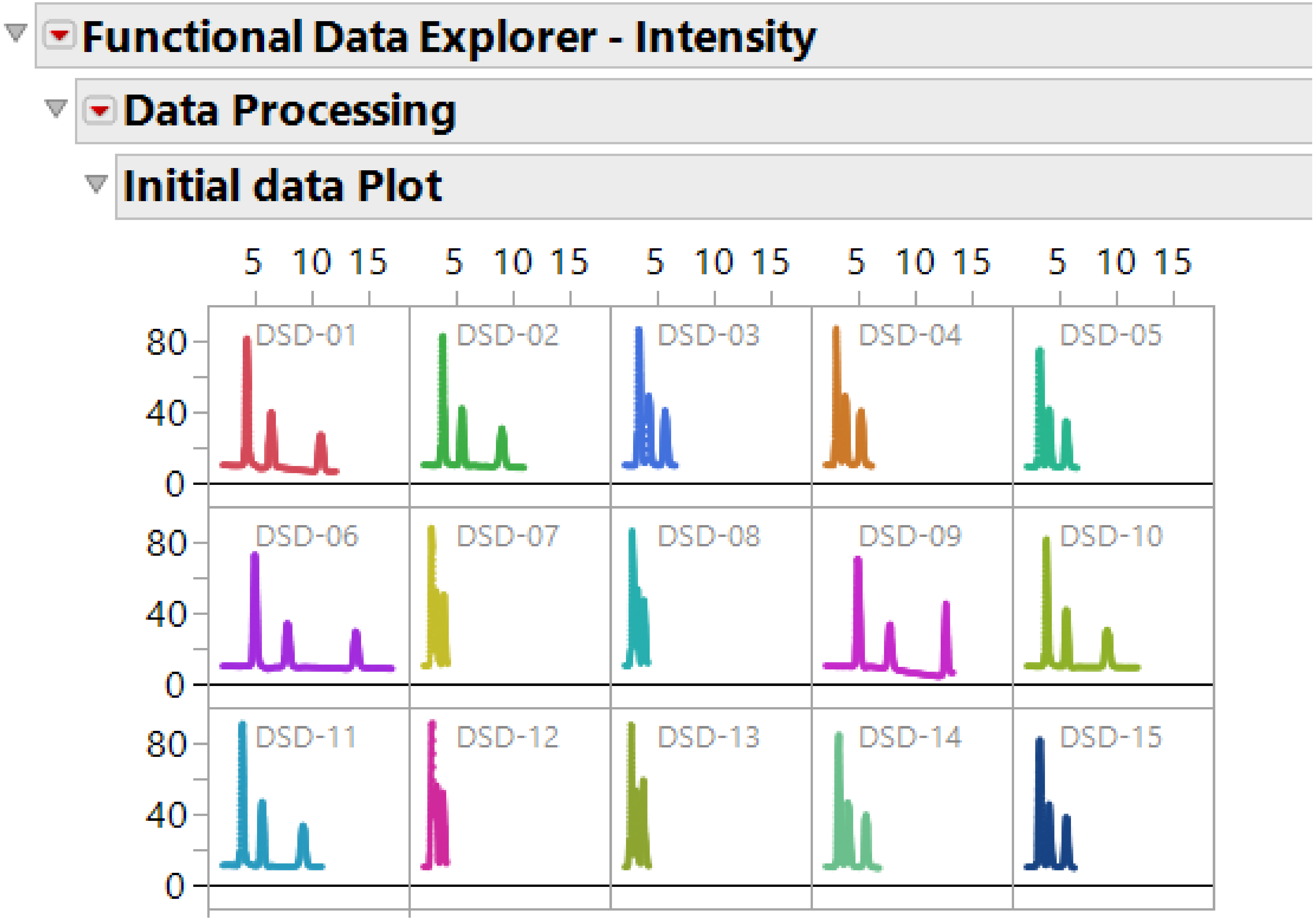

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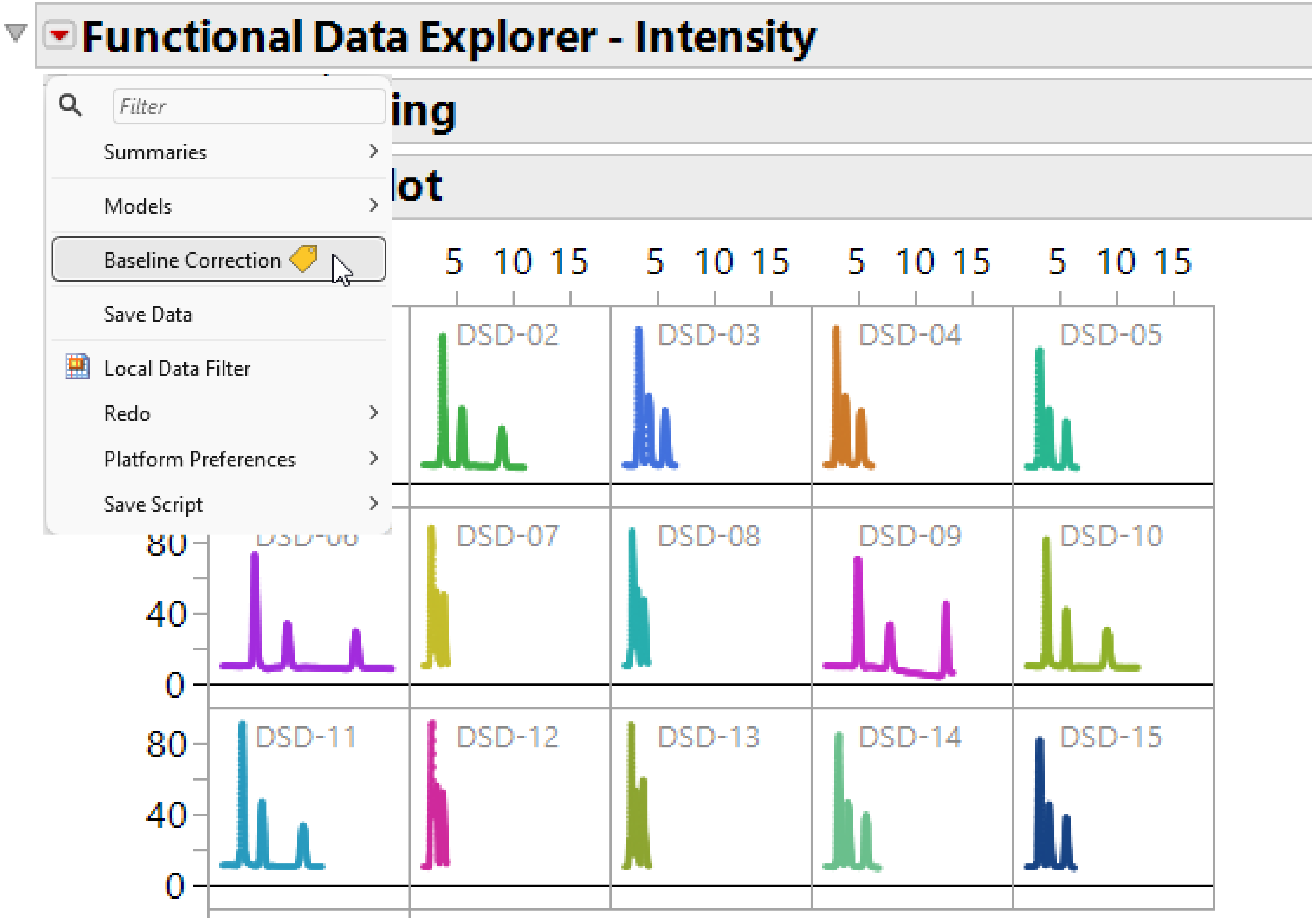

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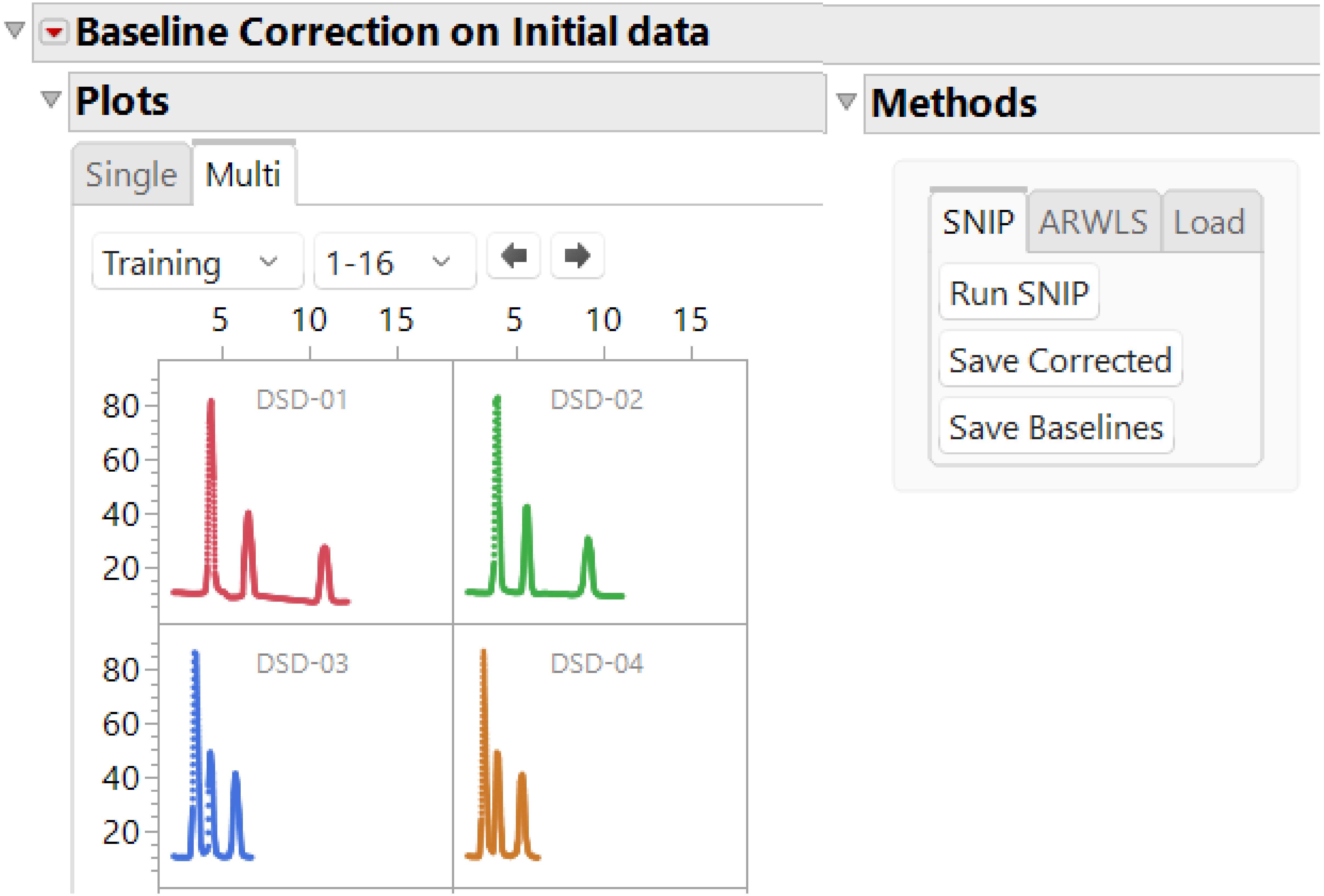

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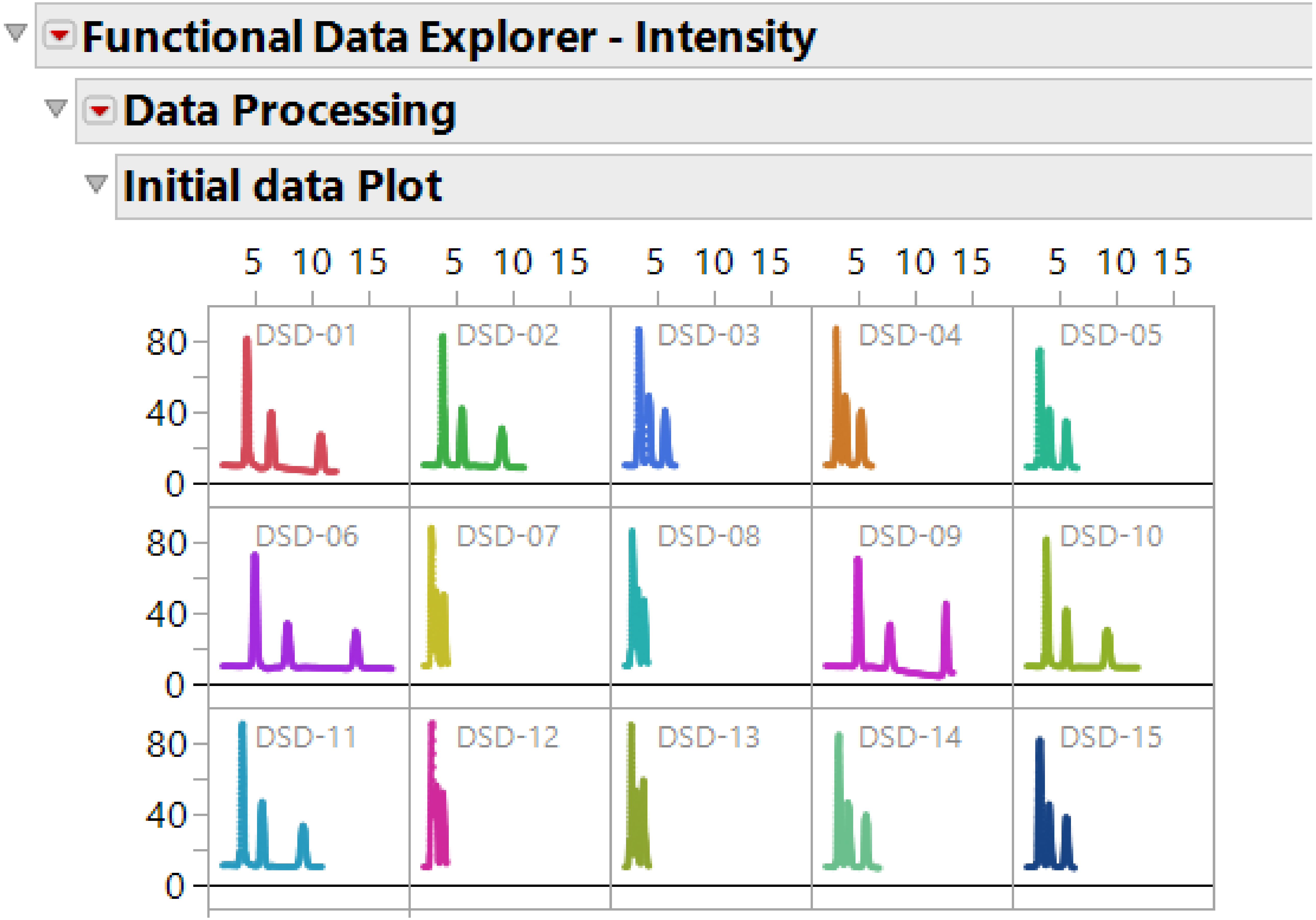

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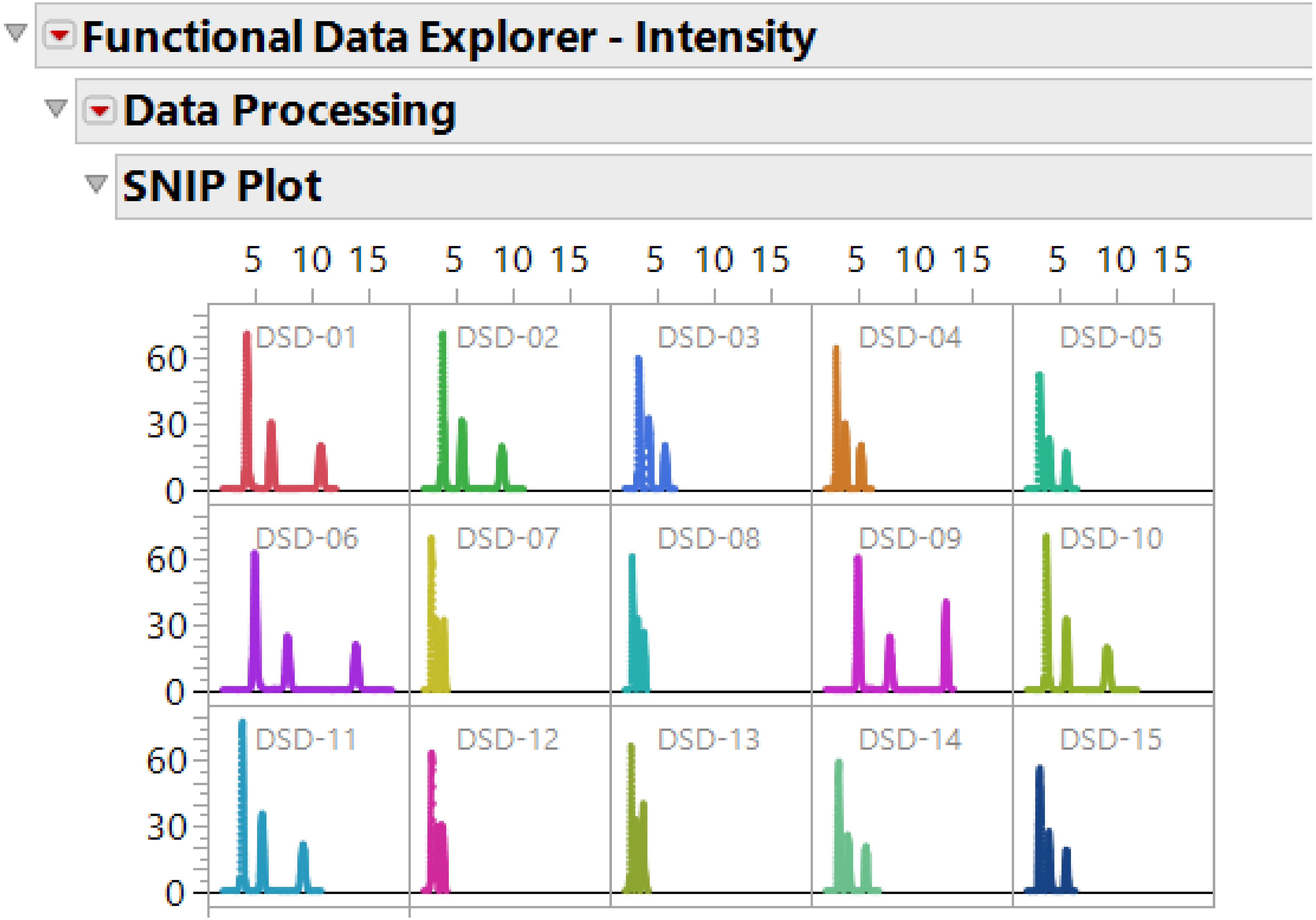

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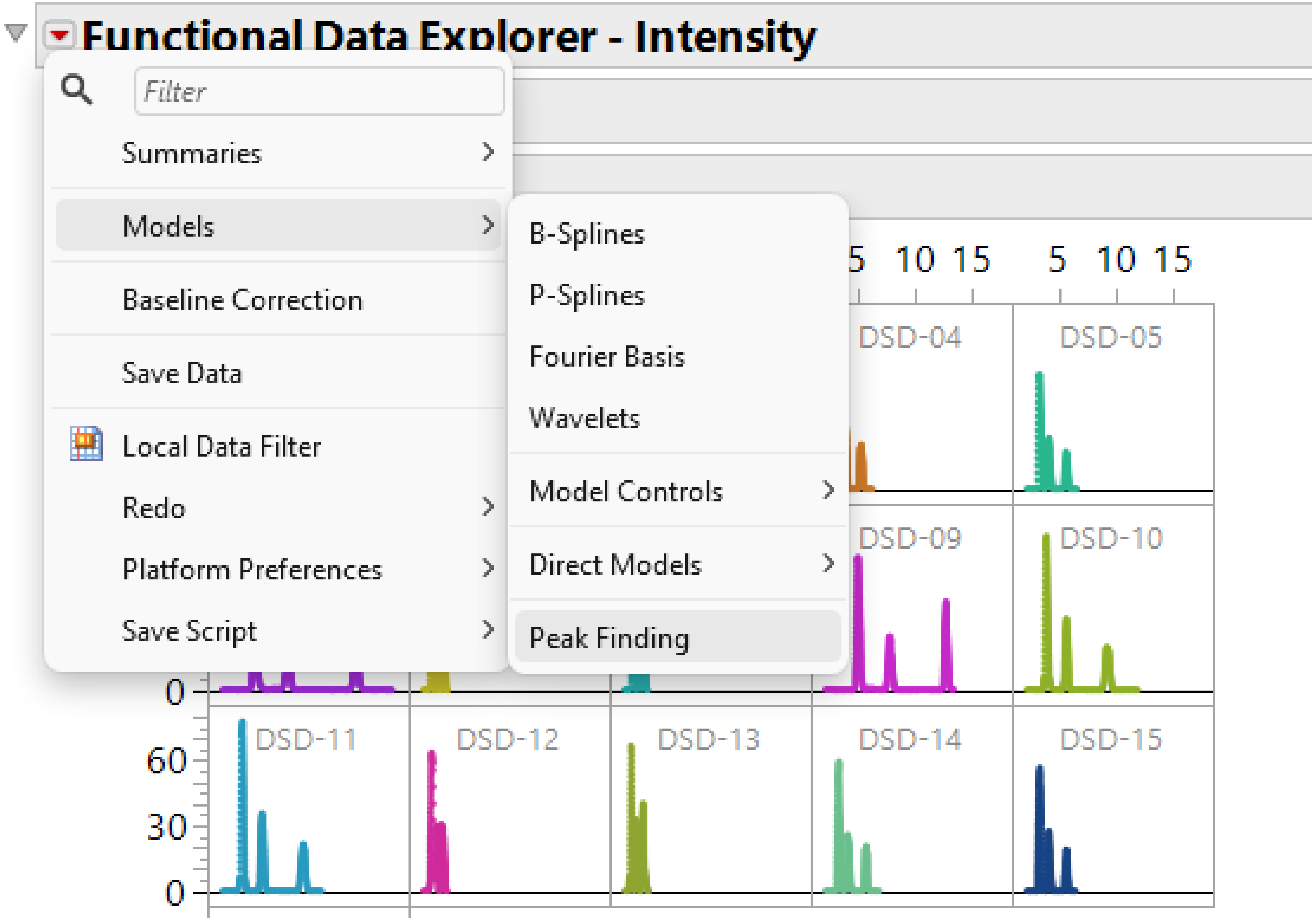

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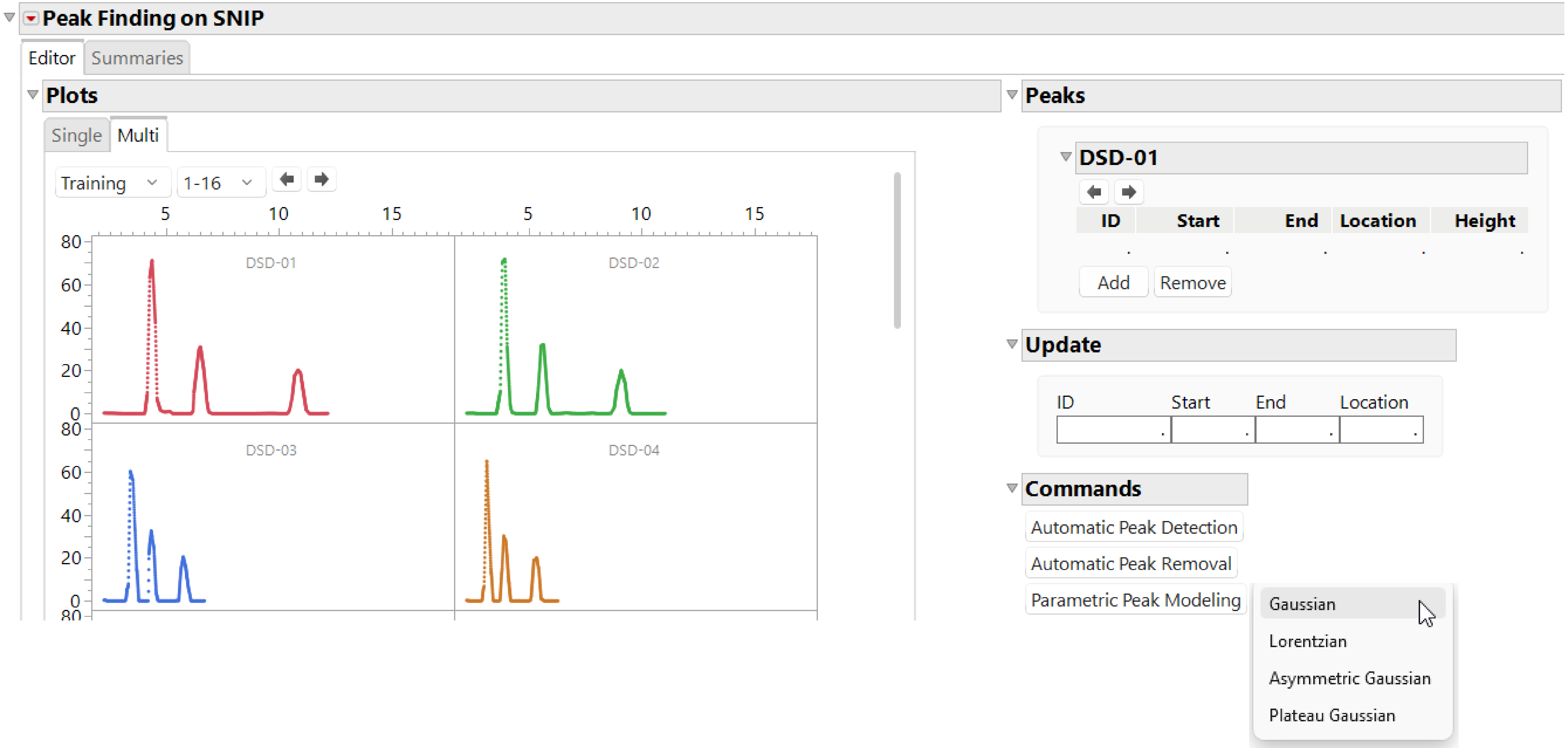

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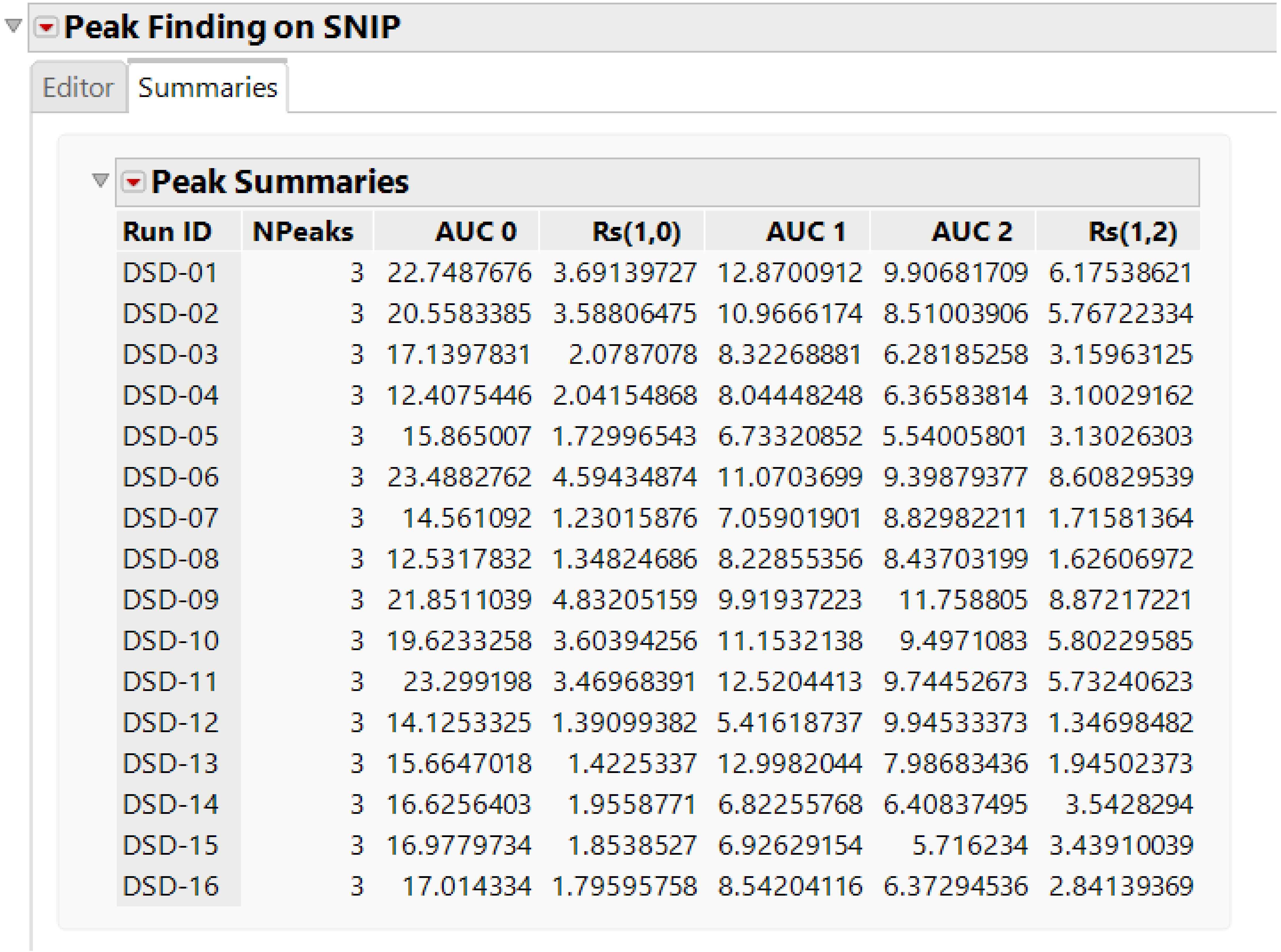


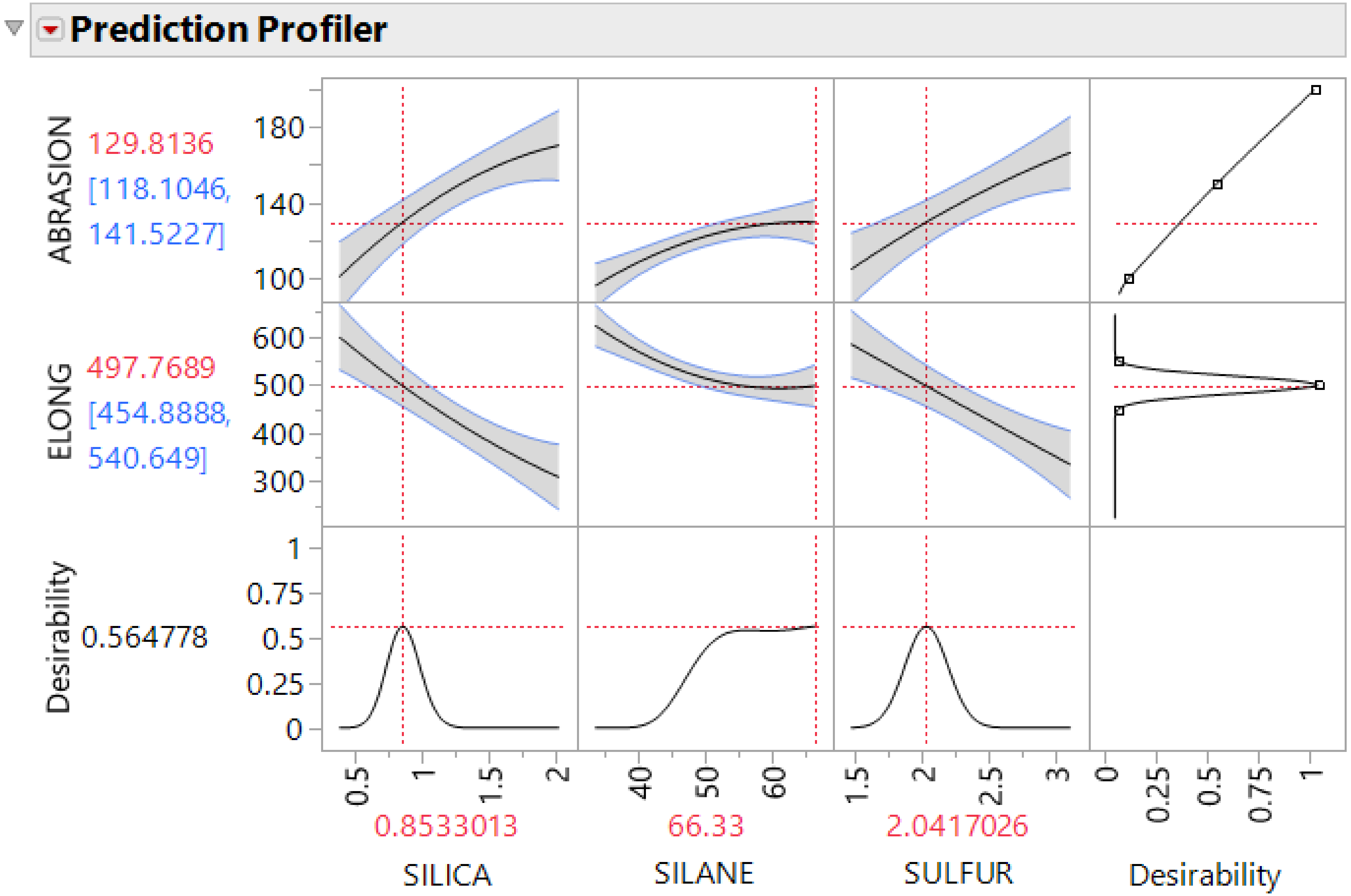
Peak Finding on SNIP

Peak Summaries

Run ID	NPeaks	AUC 0	Rs(1,0)	AUC 1	AUC 2	Rs(1,2)
DSD-01	3	22.7487676	3.69139727	12.8700912	9.90681709	6.17538621
DSD-02	3	20.5583385	3.58806475	10.9666174	8.51003906	5.76722334
DSD-03	3	17.1397831	2.0787078	8.32268881	6.28185258	3.15963125
DSD-04	3	12.4075446	2.04154868	8.04448248	6.36583814	3.10029162
DSD-05	3	15.865007	1.72996543	6.73320852	5.54005801	3.13026303
DSD-06	3	23.4882762	4.59434874	11.0703699	9.39879377	8.60829539
DSD-07	3	14.561092	1.23015876	7.05901901	8.82982211	1.71581364
DSD-08	3	12.5317832	1.34824686	8.22855356	8.43703199	1.62606972
DSD-09	3	21.8511039	4.83205159	9.91937223	11.758805	8.87217221
DSD-10	3	19.6233258	3.60394256	11.1532138	9.4971083	5.80229585
DSD-11	3	23.299198	3.46968391	12.5204413	9.74452673	5.73240623
DSD-12	3	14.1253325	1.39099382	5.41618737	9.94533373	1.34698482
DSD-13	3	15.6647018	1.4225337	12.9982044	7.98683436	1.94502373
DSD-14	3	16.6256403	1.9558771	6.82255768	6.40837495	3.5428294
DSD-15	3	16.9779734	1.8538527	6.92629154	5.716234	3.43910039
DSD-16	3	17.014334	1.79595758	8.54204116	6.37294536	2.84139369

Bayesian Optimization

Bayesian Optimization



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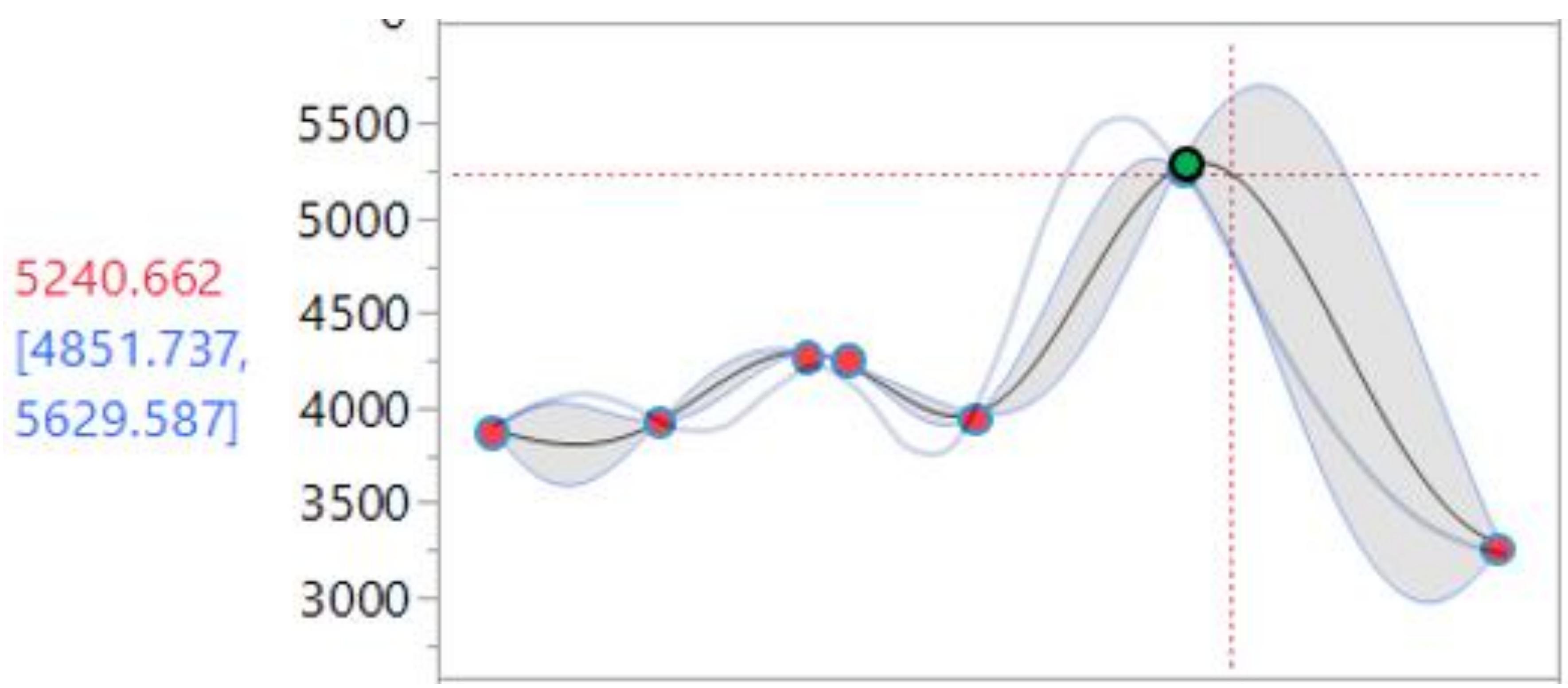
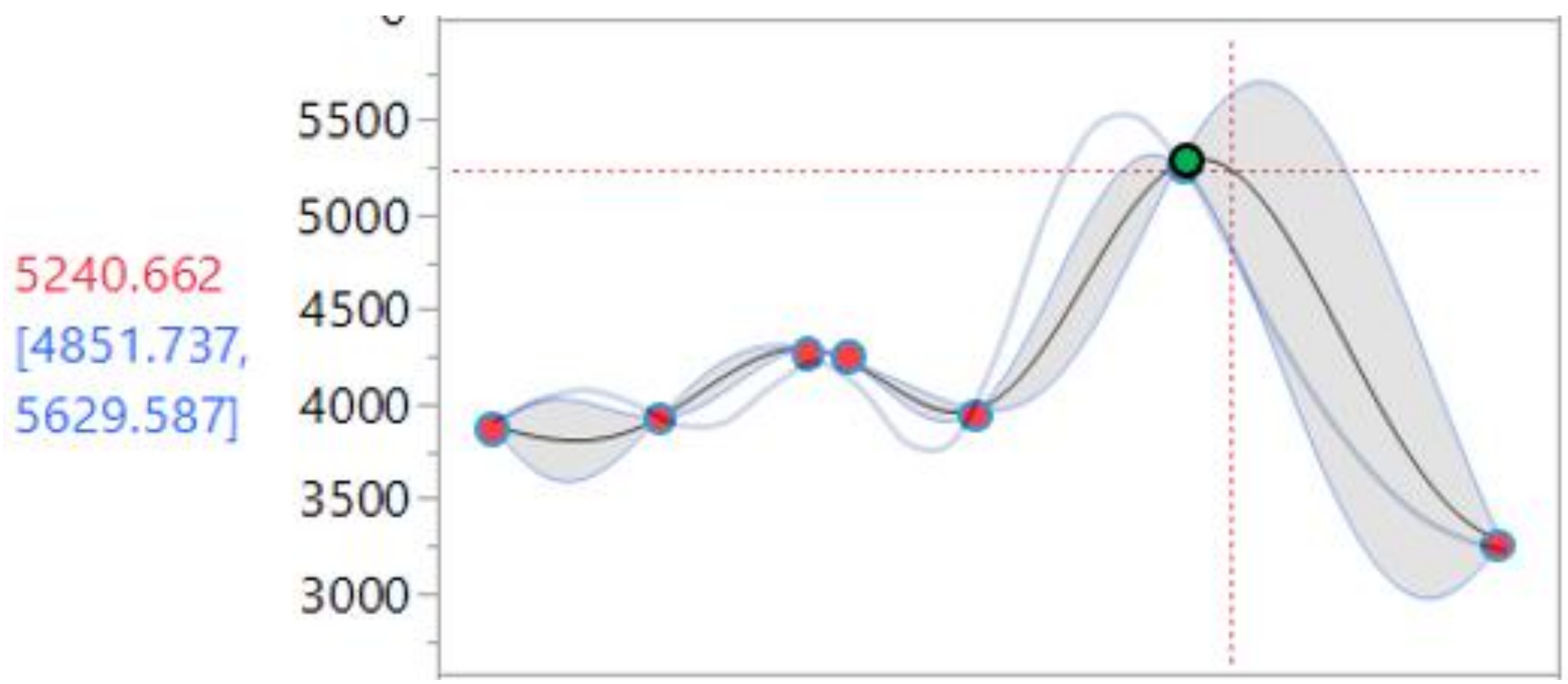


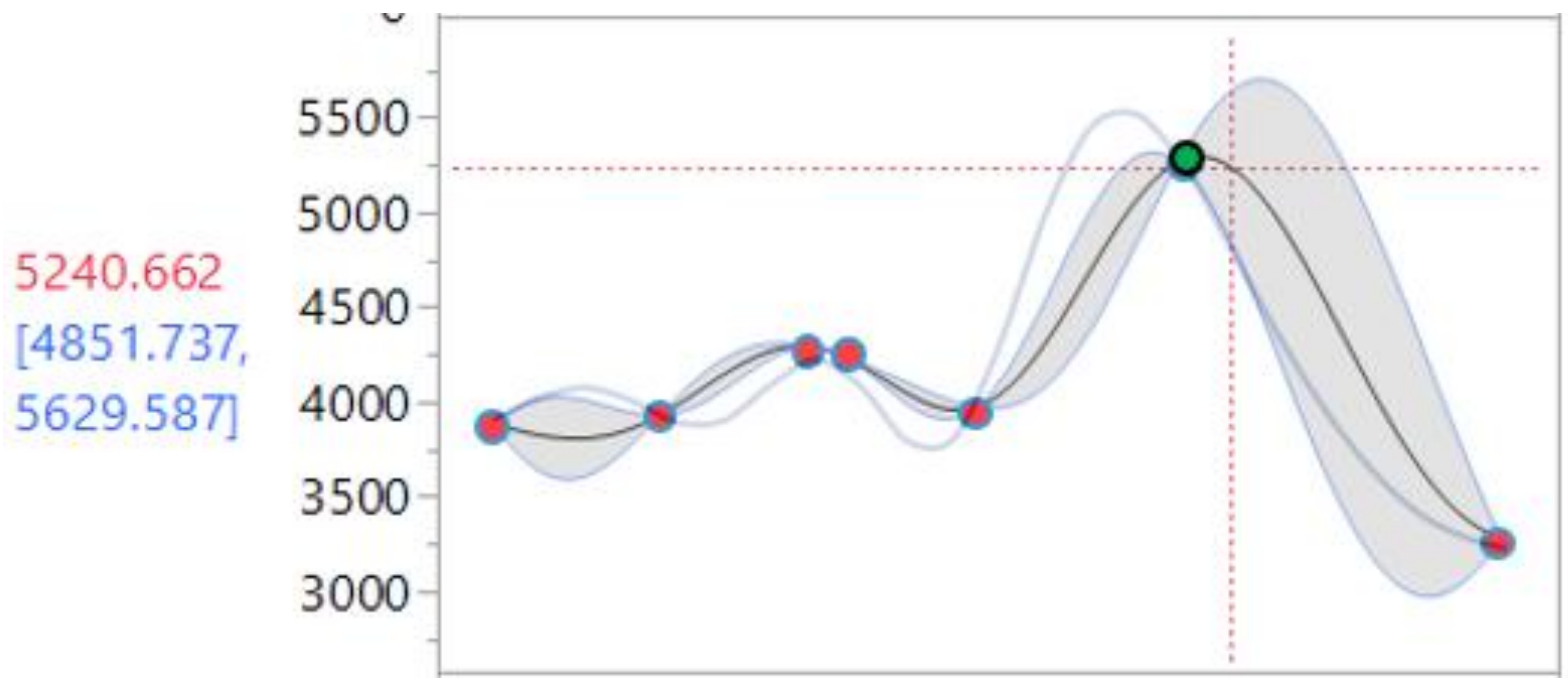
- ***Flexible to work the way you want to:***
    - Recommends small batches that adapt to your production process
    - Easy to incorporate ad-hoc proposals
    - Easy to change ranges and add variables
    - Easy to fix factors, optimize others: “smart OFAT”
    - Easy mixture/constraint handling

Bayesian Optimization



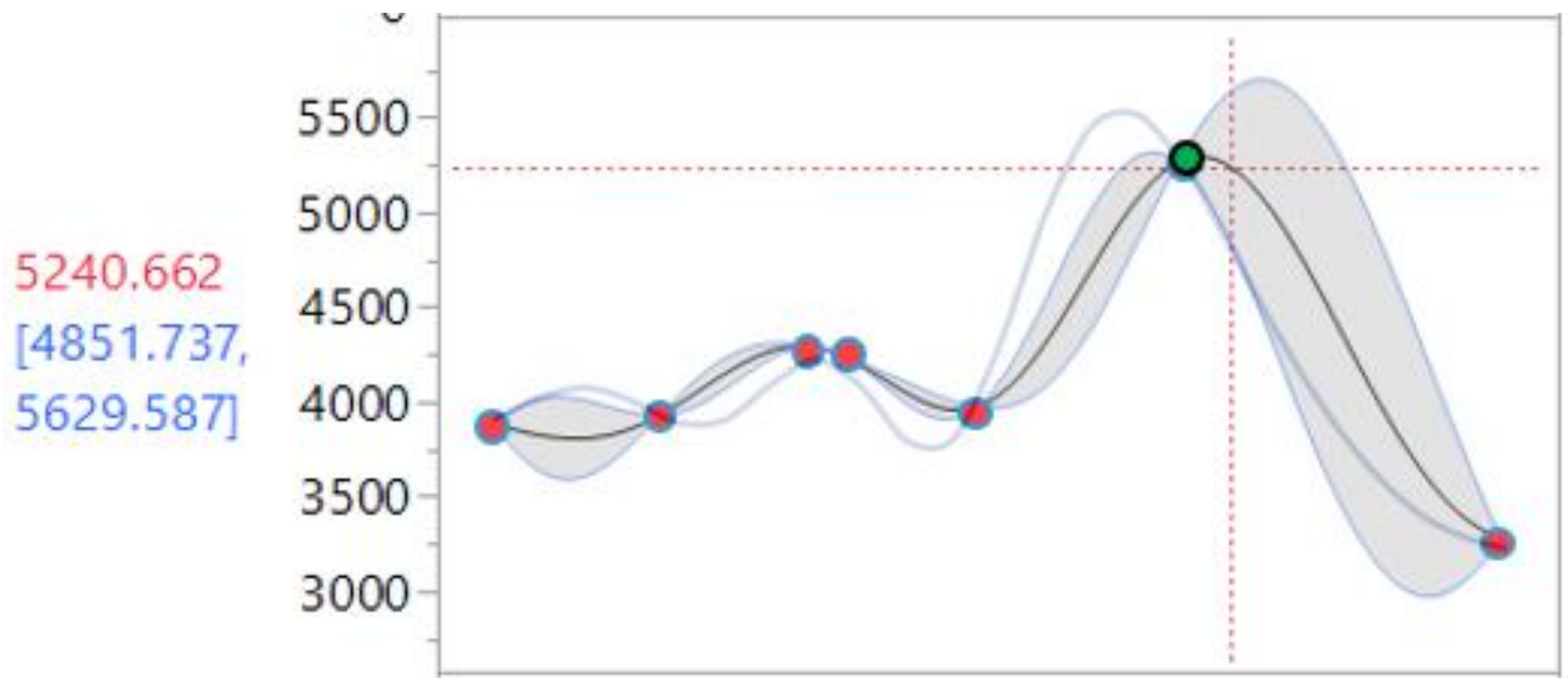
- ***Faster and more efficient:***
  - Small starting data (8 factors, 2 starting runs!)
  - Use messy initial starting data
  - Work iteratively and stop when goals are met
  - Using responses and goals accelerates innovation

Bayesian Optimization



- ***Problem solving without the statistical machinery:***
    - No p-values, hypothesis tests, or power calcs
    - Response surface emerges directly from the data
    - No interaction or curvature effects to declare
    - No such thing as VIFs, less concern about aliasing
    - Randomization often the opposite of what you want

Bayesian Optimization



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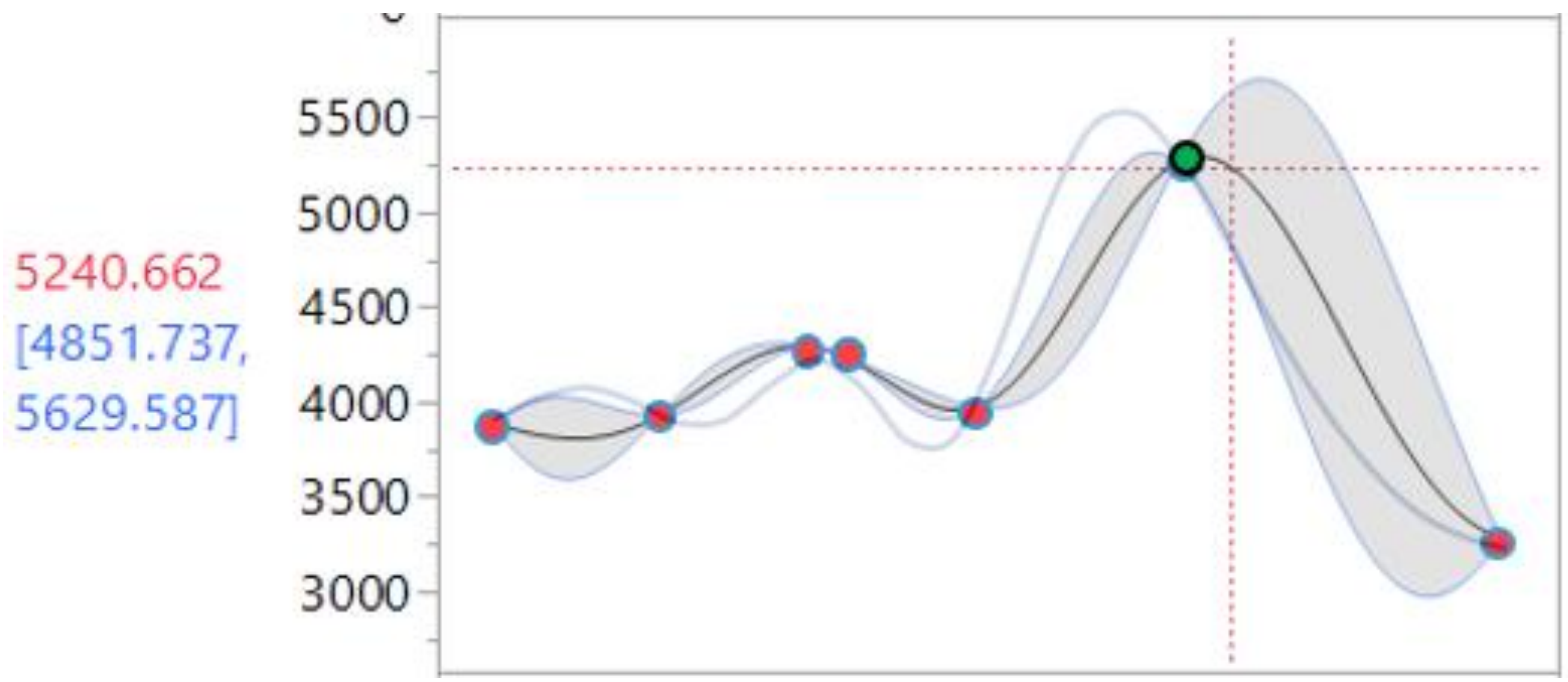
Statistical analysis is about ***proving things,*** Bayesian optimization is about **improving things**

Bayesian Optimization



"***Basic Bayesian Optimization***"

- Maximize a single response, $\mathrm{y(x)}$
  - Inputs, x, are continuous
  - $\mathrm{y(x)}$ observed with little / no error
- $\mathrm{y(x)}$ modeled w/ a GaSP:
  - $\mathrm{y(x)} \sim N(\mu(x), \sigma^2(x))$
- Recommends one run at a time trading off $\mu(x)$ and $\sigma^2(x)$

“*EXOTIC*” BAYESIAN OPTIMIZATION

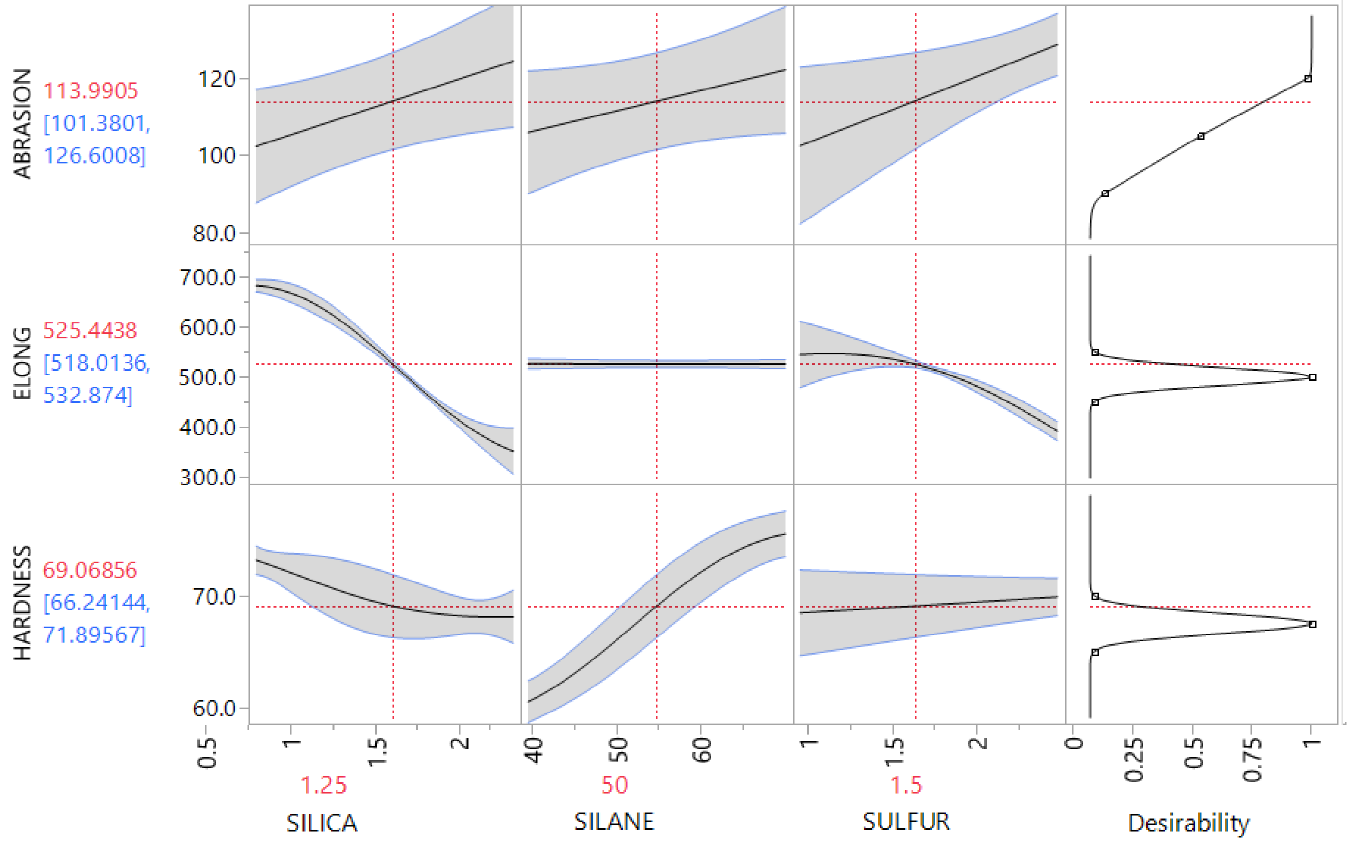
- $\mathrm{y}(x)$ observed with random error
- Categorical inputs or outputs
- Missing inputs
- “*Batch*” augmentation of more than one run
- Many inputs: $\dim(x) > 20$
- Adding new factors in middle of project

- Multiple responses, $y_i(x)$, with
  - Competing goals
  - Complicated sparsity
- Match target/spec limit goal
  - $\mathrm{y}(x) = Y_T$ or $\mathrm{y}(x) \in [Y_L, Y_U]$
- Randomization restrictions (blocking & split plotting)
- Messy training data of unknown and dubious value

Bayesian Optimization

Every example I've seen has been "*Exotic*" in multiple ways

Bayesian Optimization



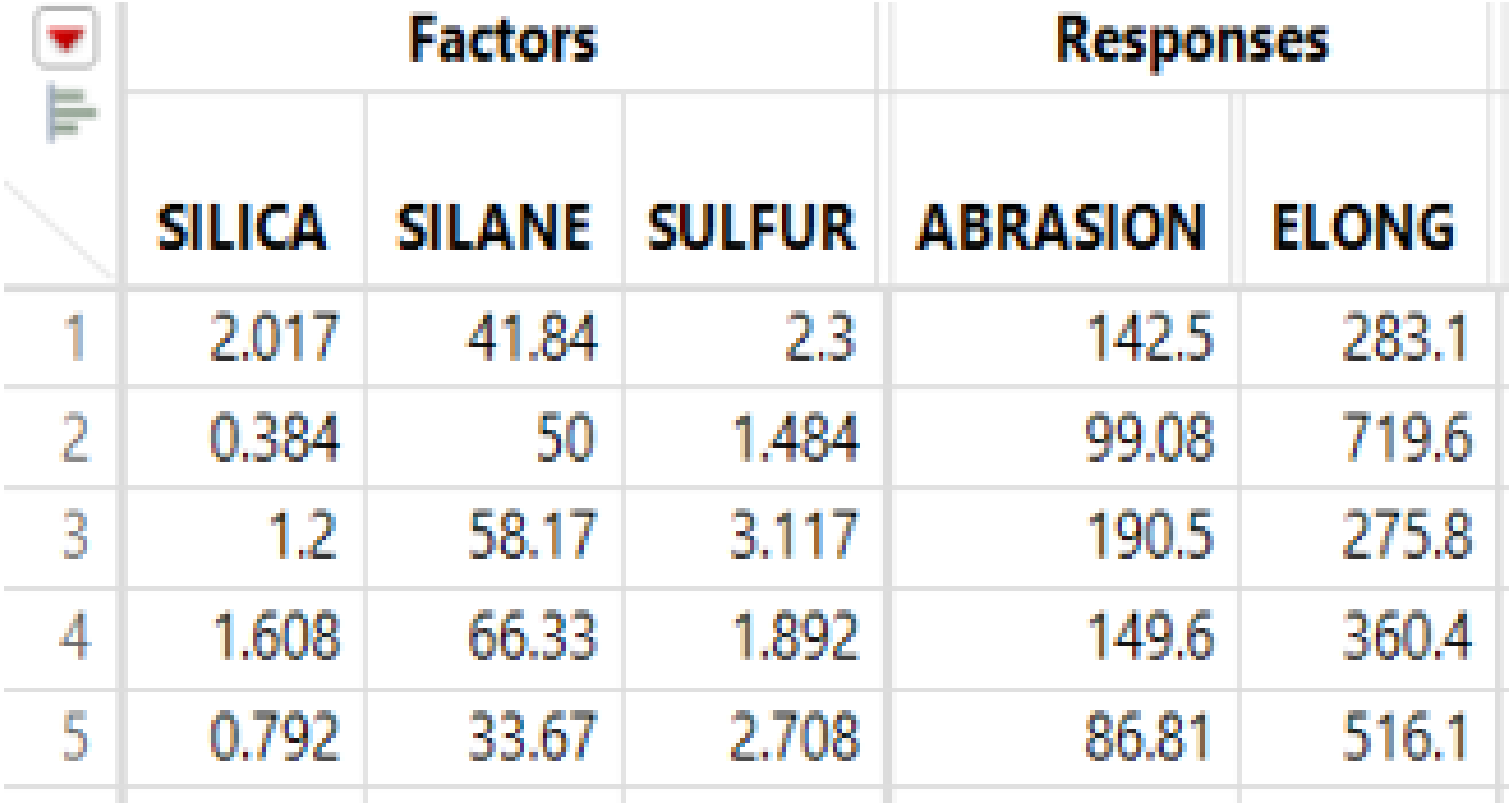
Profiler Optimization

1) Obtain DoE/Observational data.
2) Model Responses
3) Optimize response models

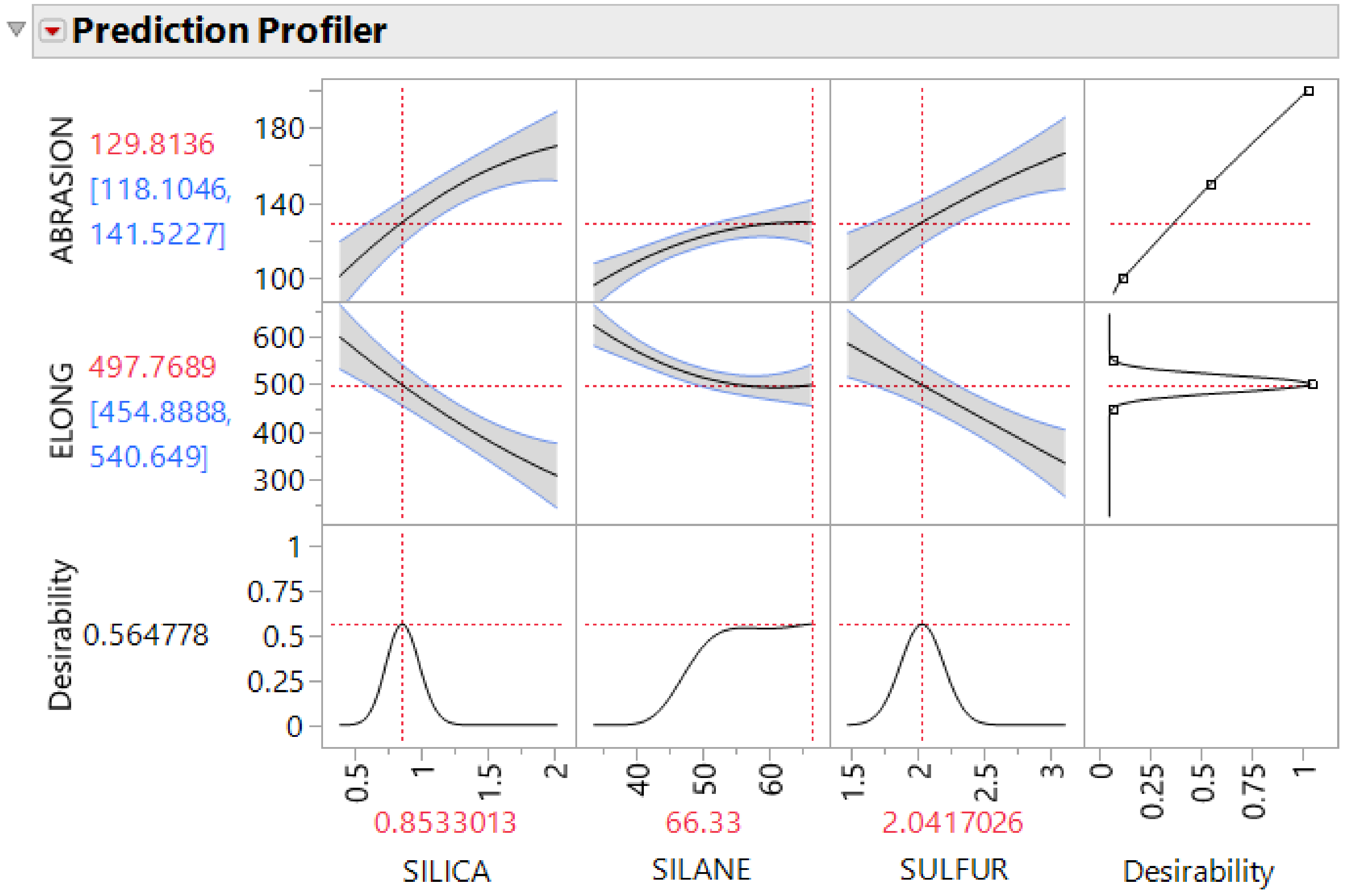
- Continuous, nominal, and ordinal x
- $y(x)$ observed with error
- Max, Min, ***and Match Target*** goals

2) x may be linearly constrained or have arbitrary Disallowed Combinations

Bayesian Optimization

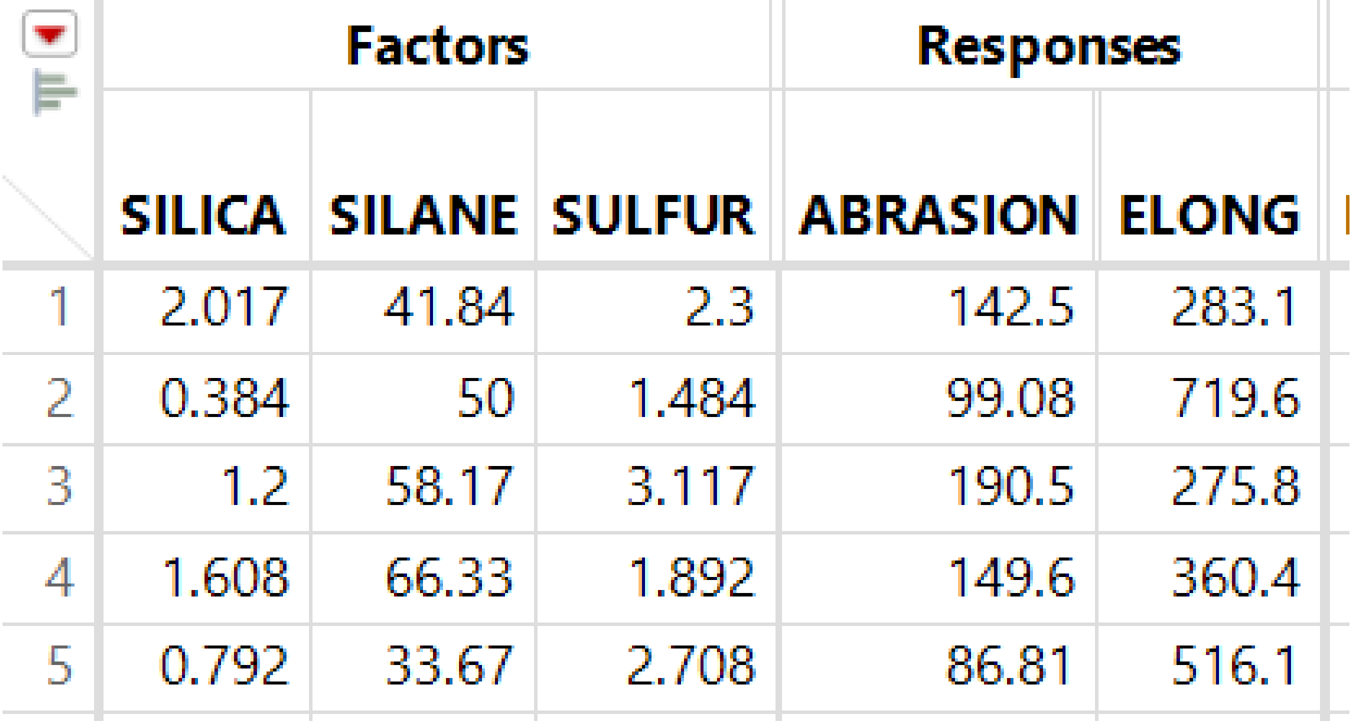


	Factors			Responses	
	SILICA	SILANE	SULFUR	ABRASION	ELONG
1	2.017	41.84	2.3	142.5	283.1
2	0.384	50	1.484	99.08	719.6
3	1.2	58.17	3.117	190.5	275.8
4	1.608	66.33	1.892	149.6	360.4
5	0.792	33.67	2.708	86.81	516.1



Bayesian Optimization

Input &
Output Data



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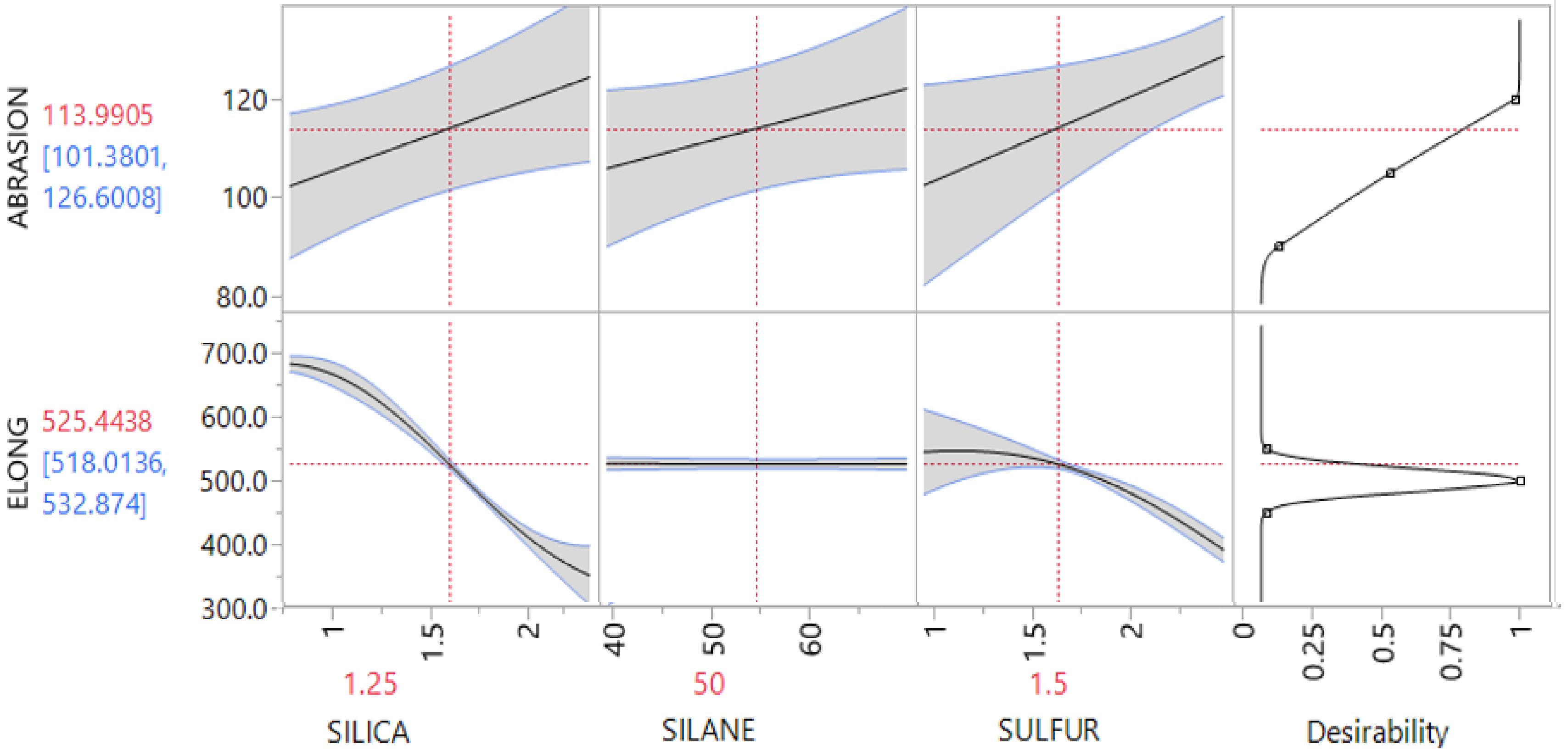

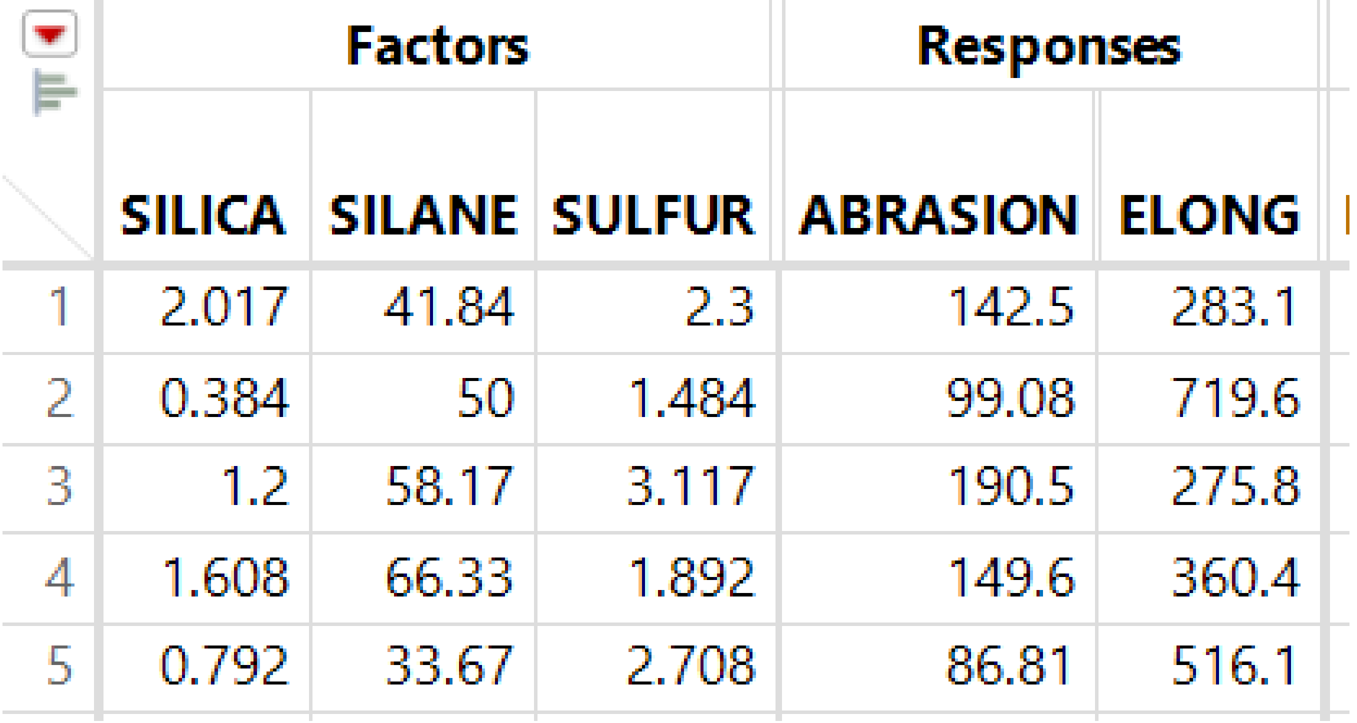

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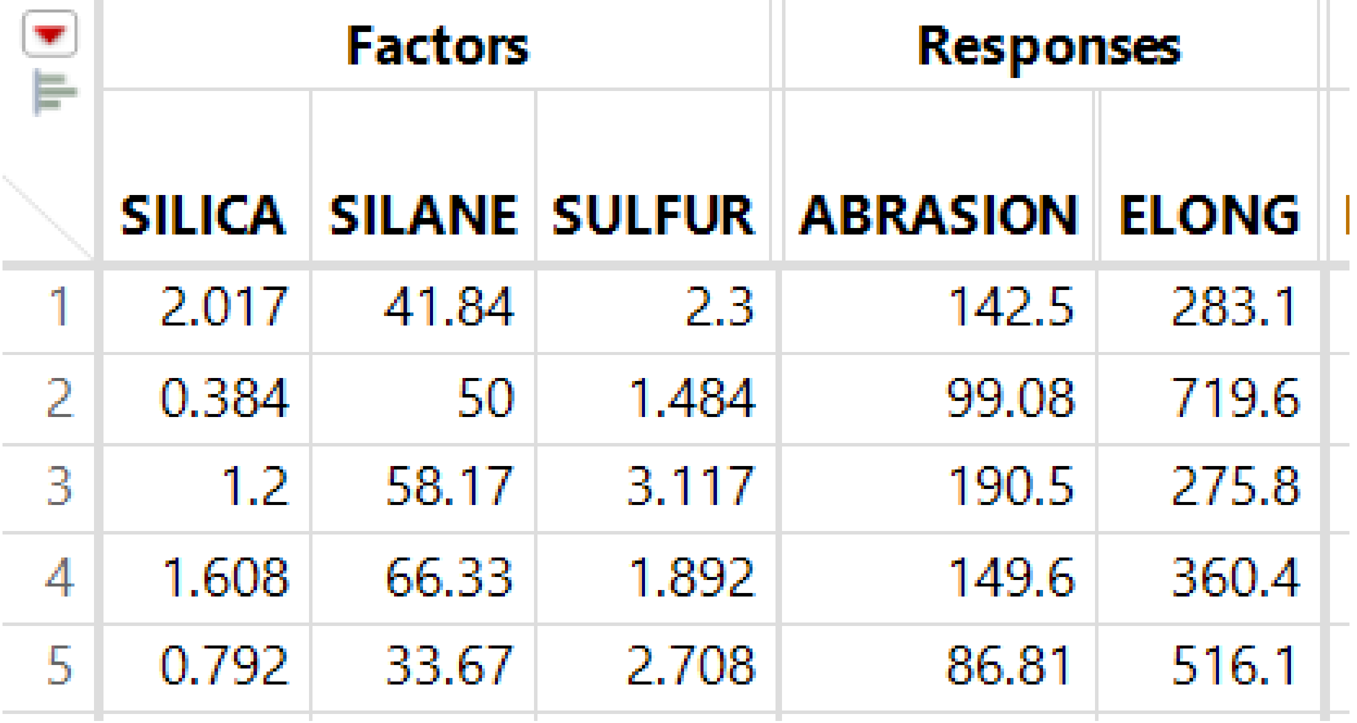

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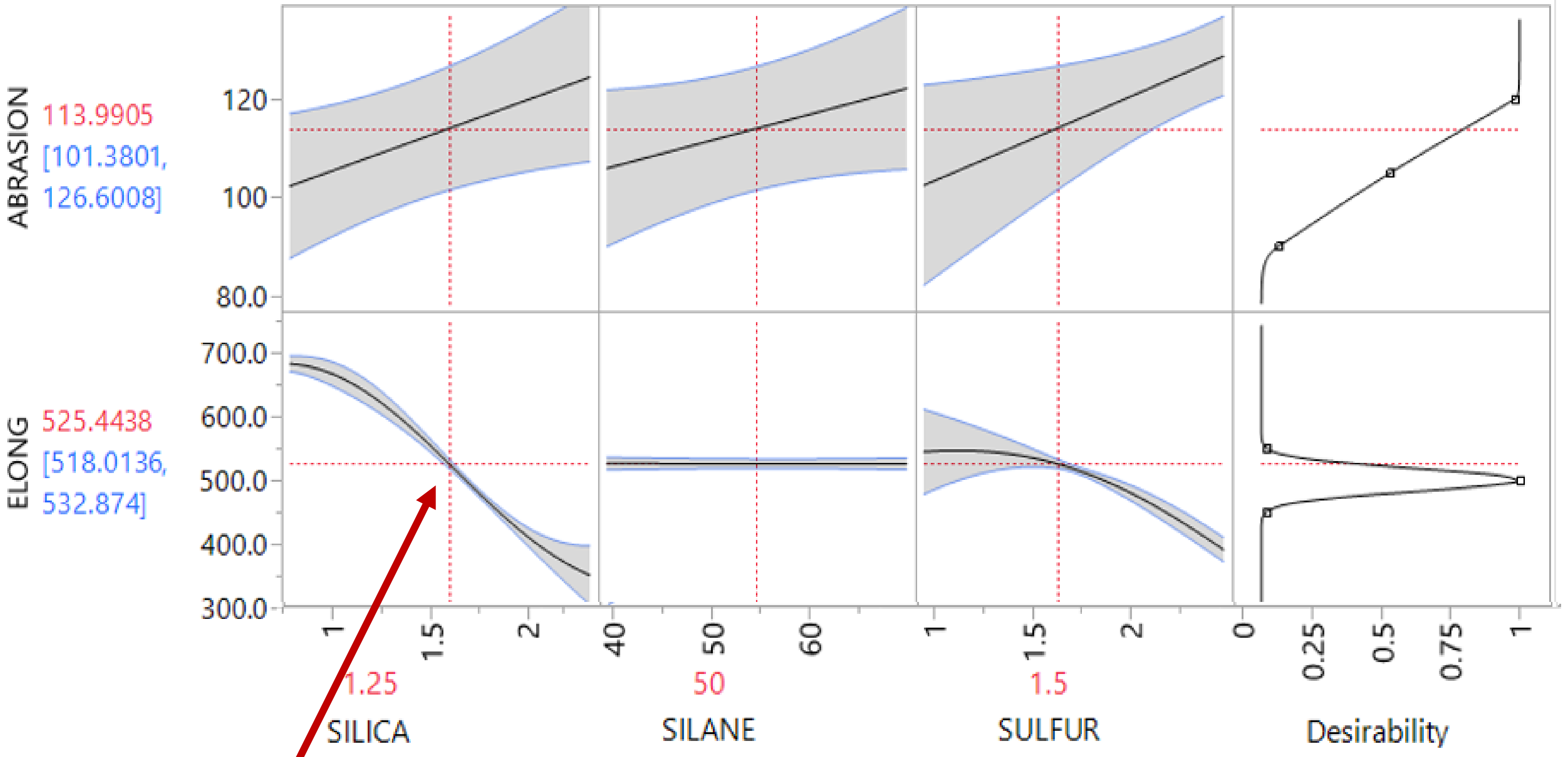
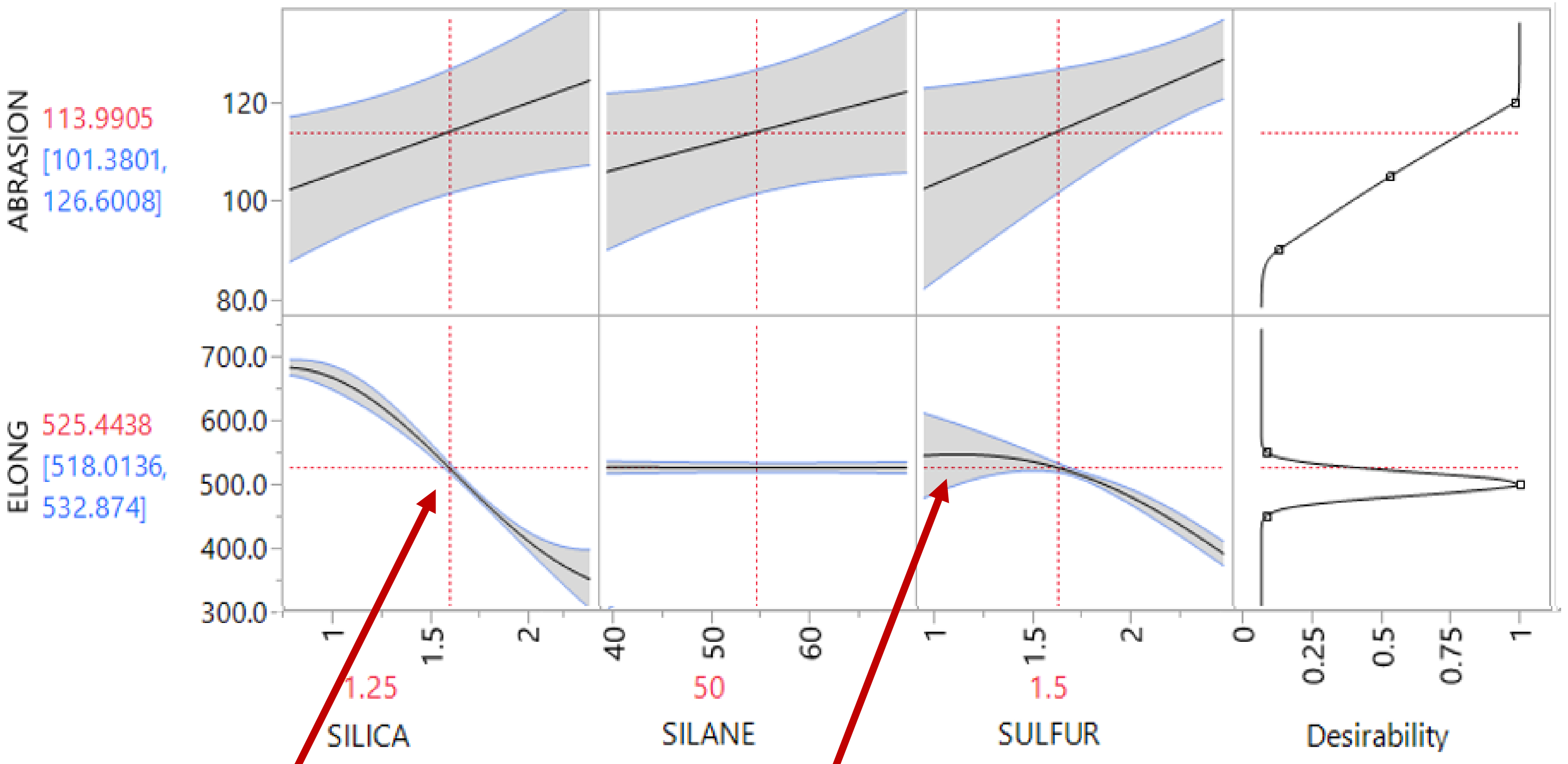
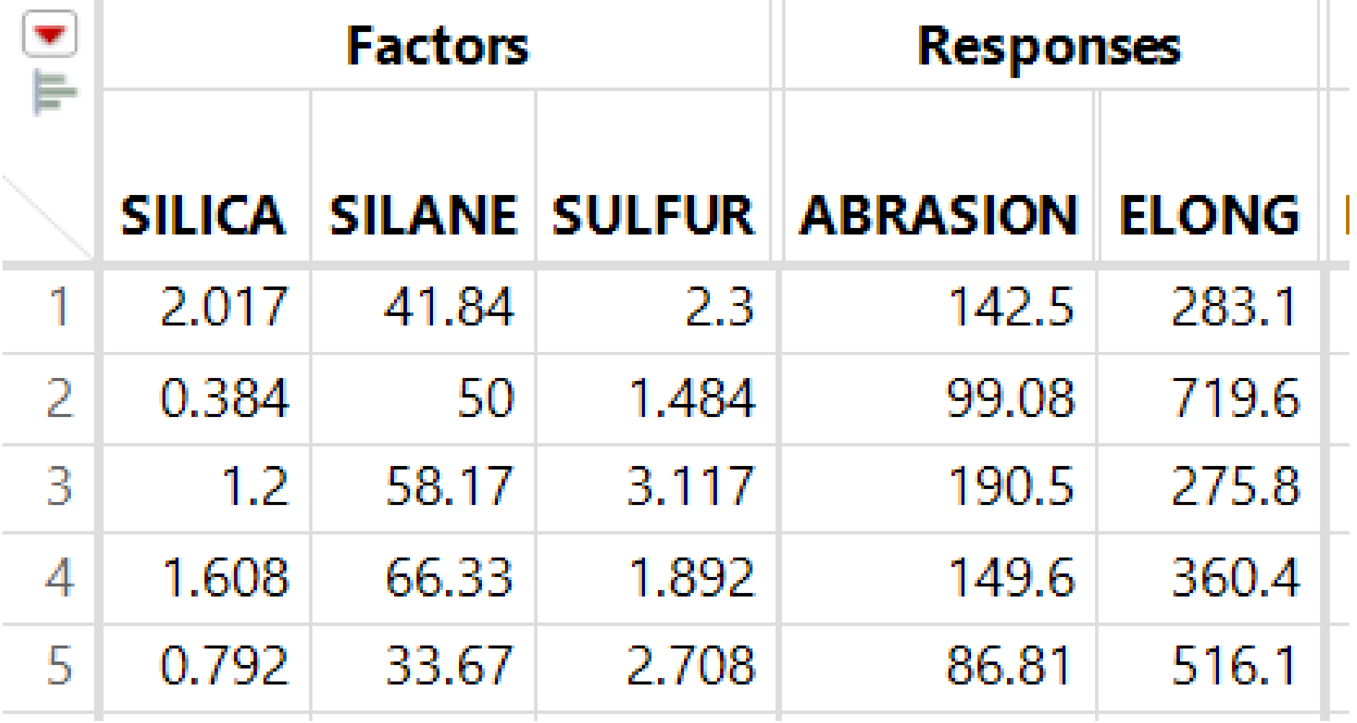


Model
Predictions

Bayesian Optimization

Input &
Output Data





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Model
Predictions

+

Prediction
Uncertainty

Bayesian Optimization

Input &
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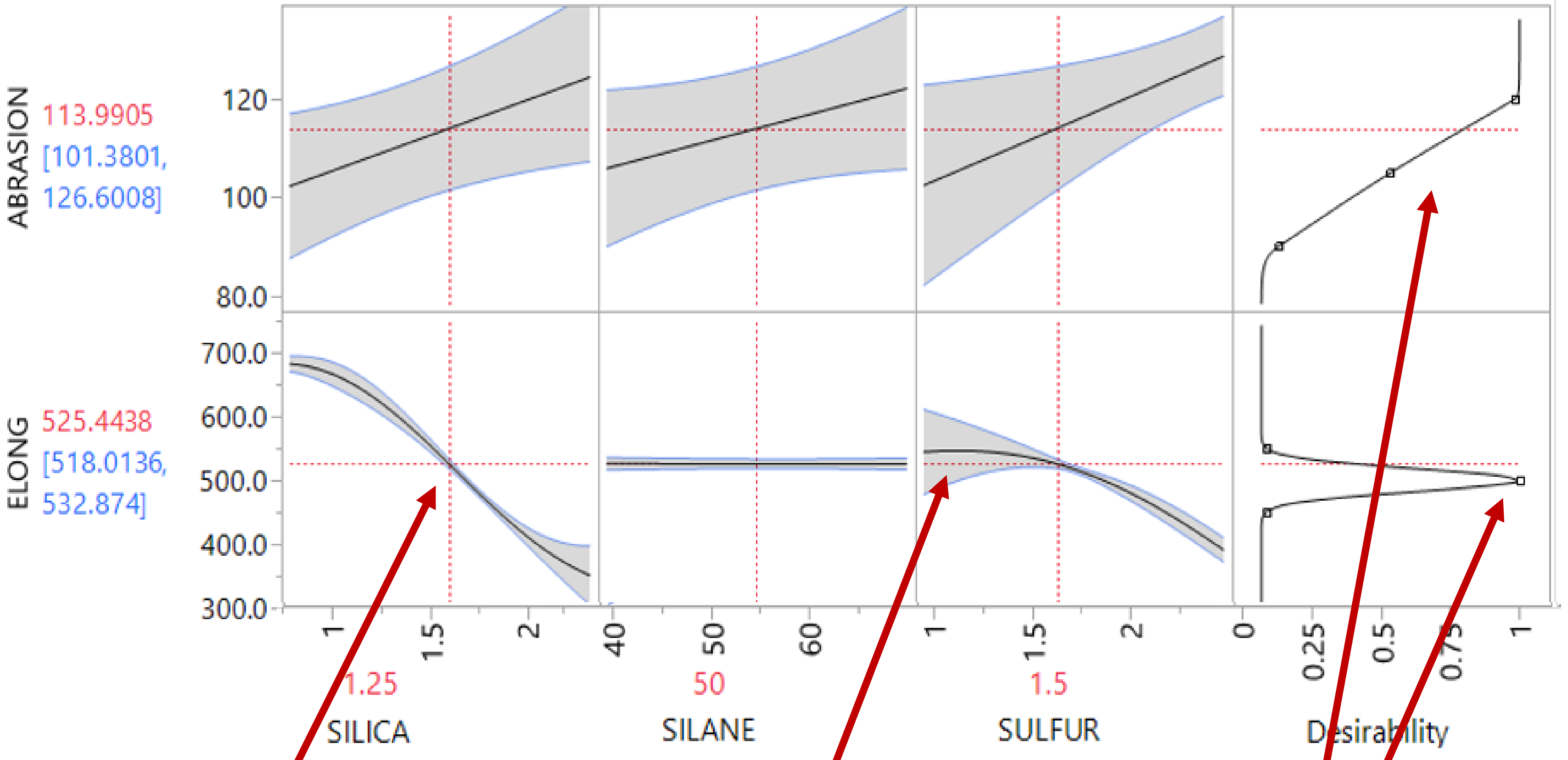

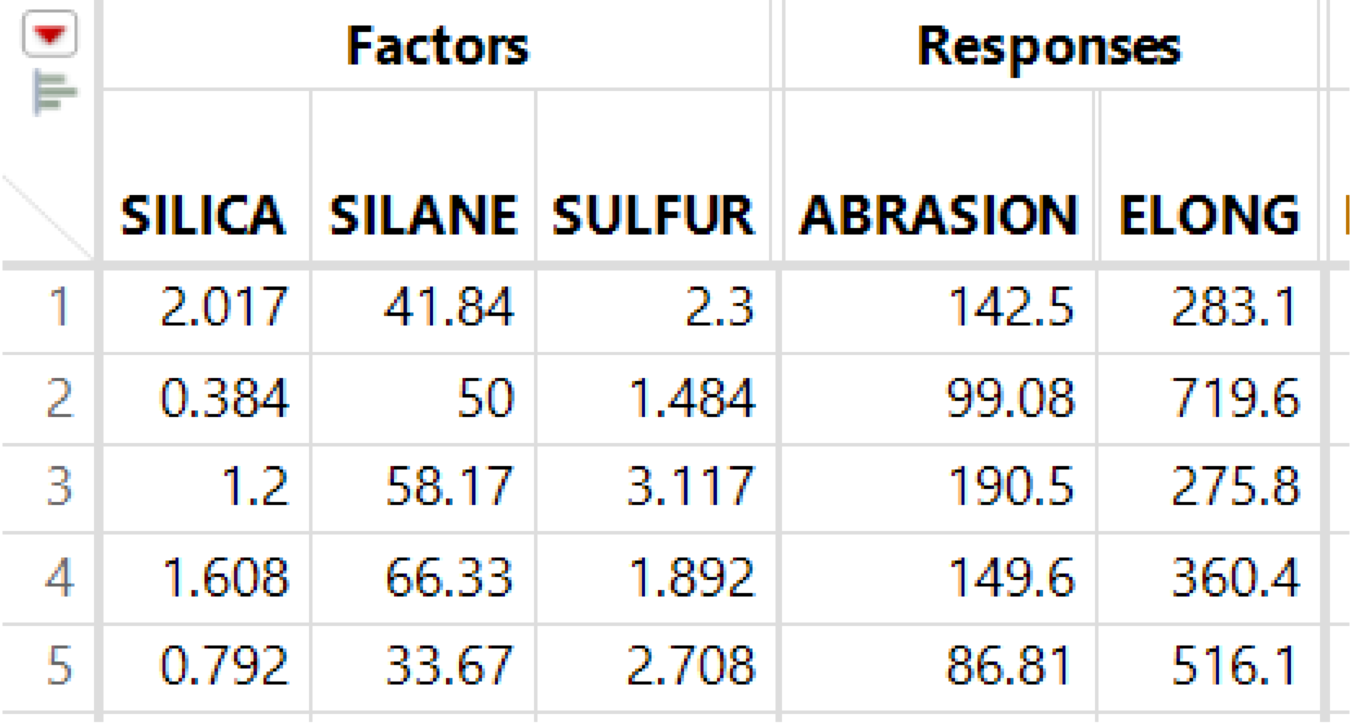

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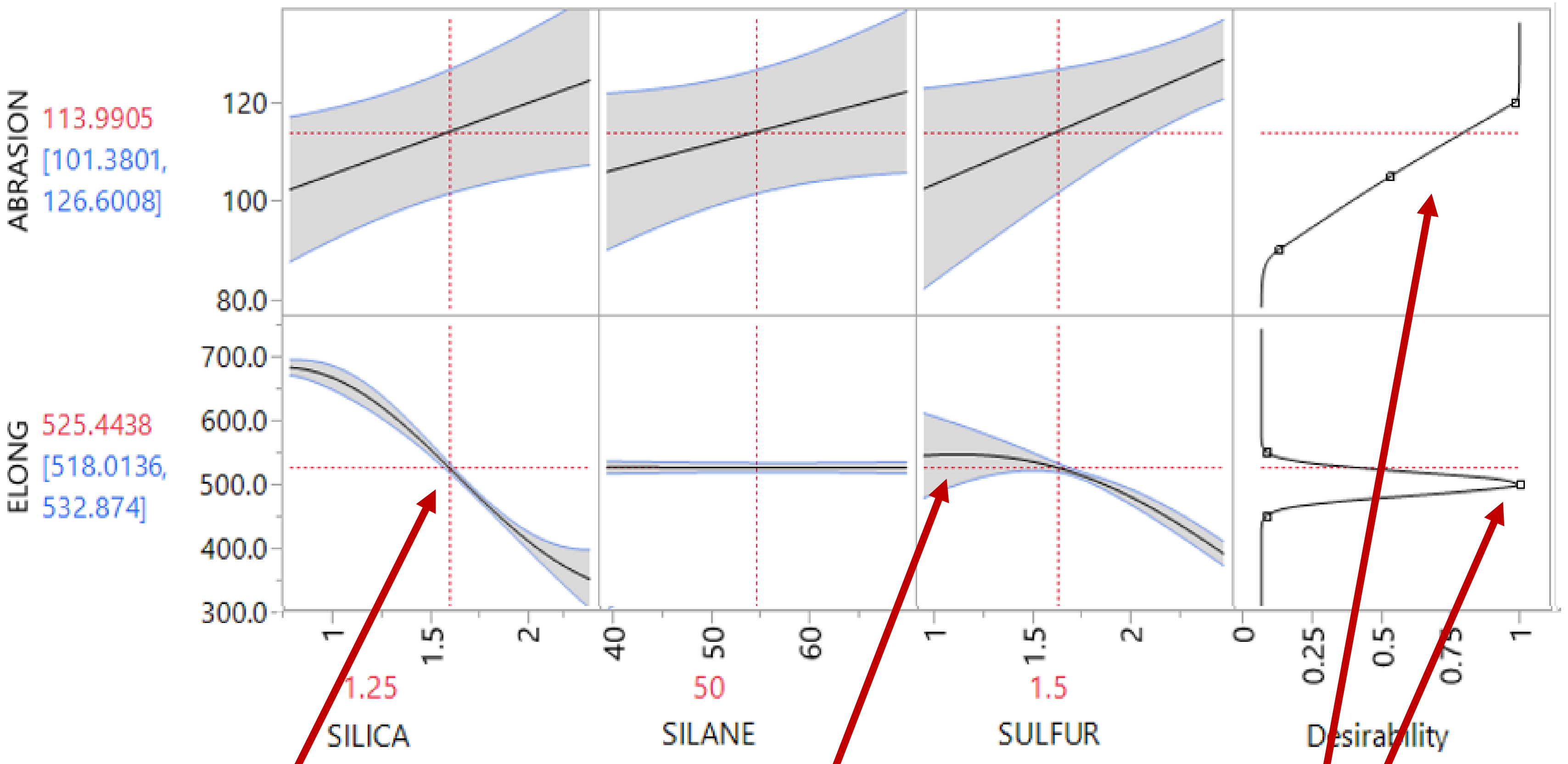
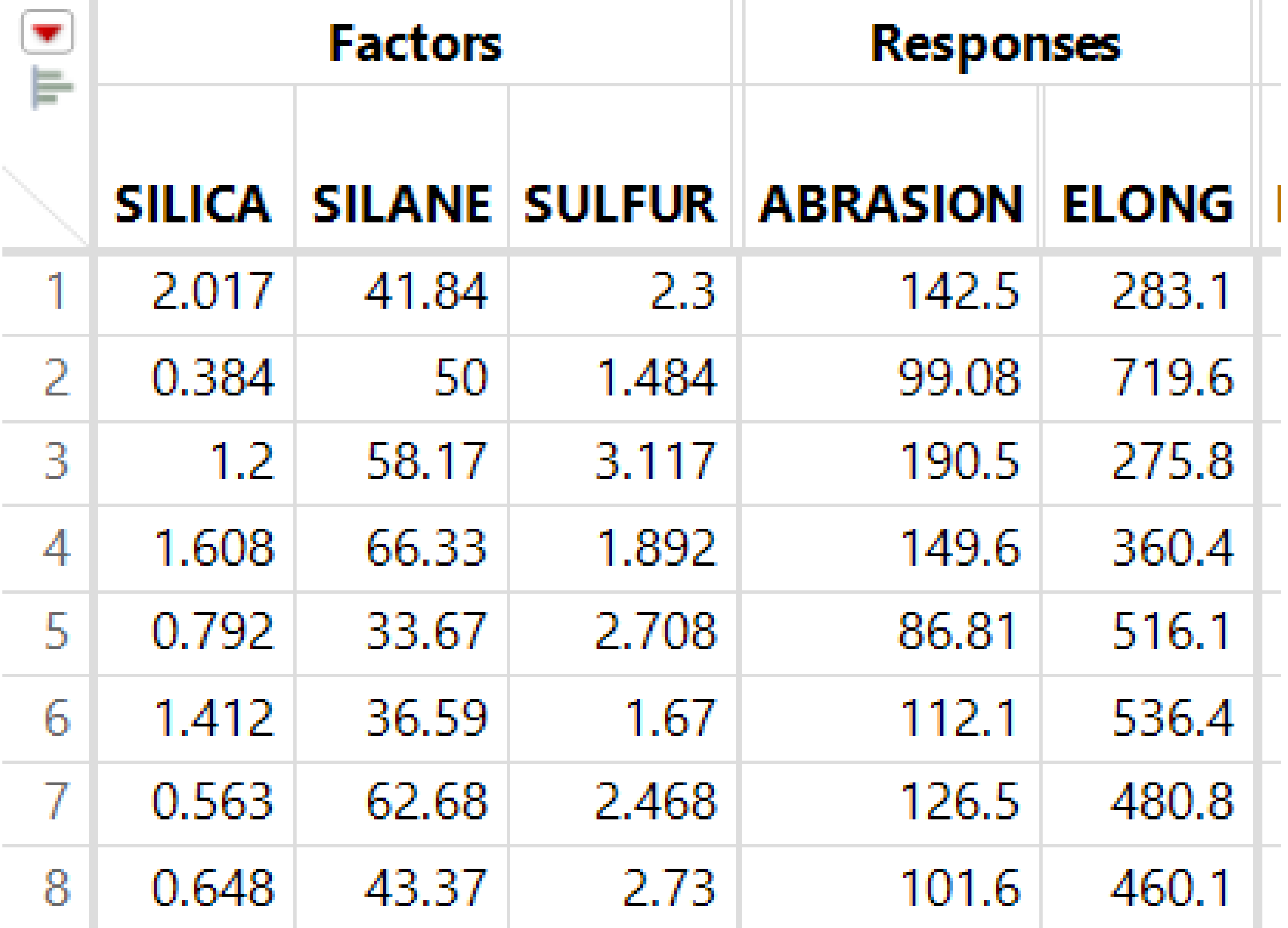
Model
Predictions + Prediction
Uncertainty + Project
Goals

Bayesian Optimization

Input &
Output Data





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5	0.792	33.67	2.708	86.81	516.1
6	1.412	36.59	1.67	112.1	536.4
7	0.563	62.68	2.468	126.5	480.8
8	0.648	43.37	2.73	101.6	460.1

Model
Predictions

\+

Prediction
Uncertainty

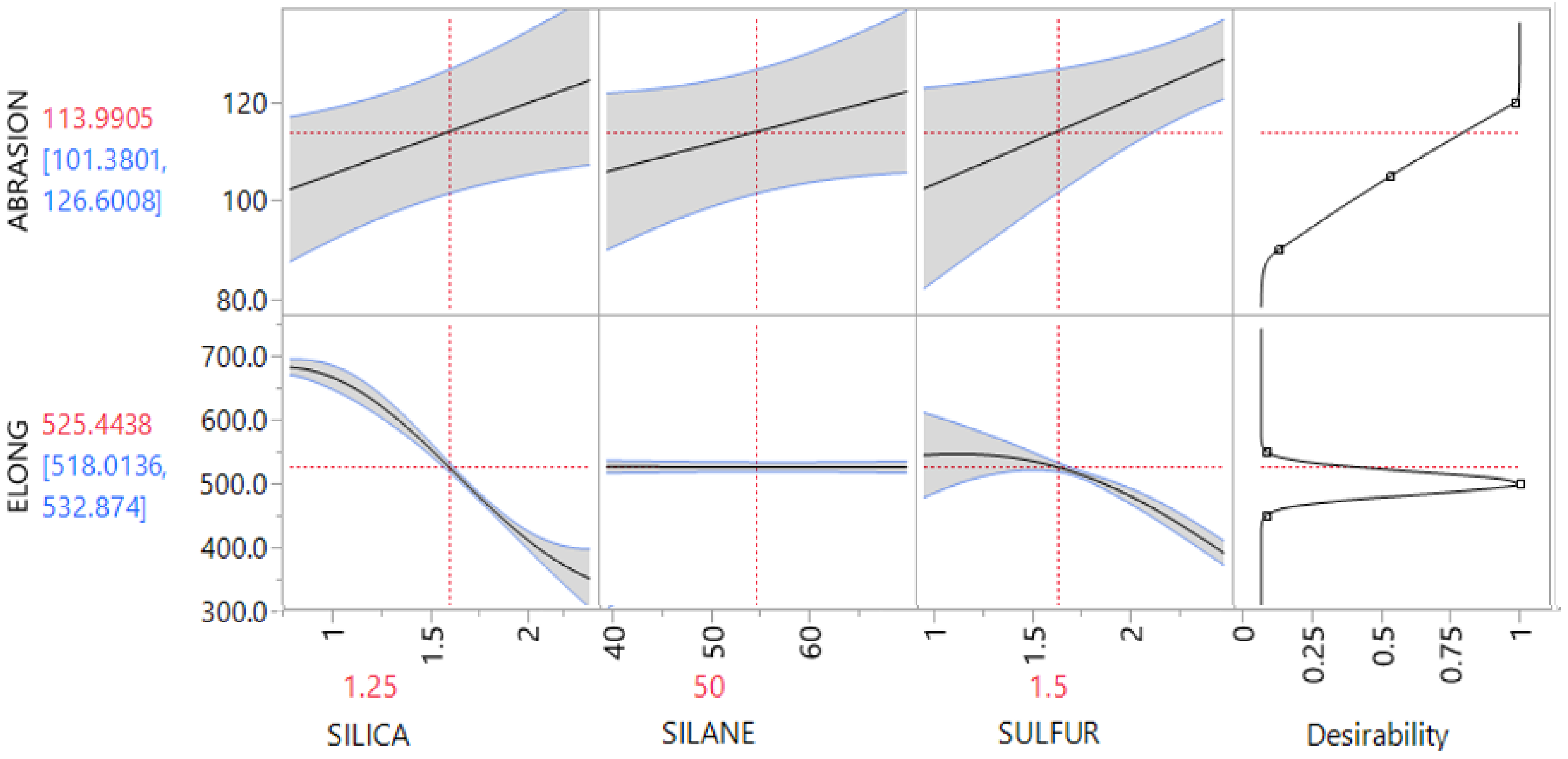
\+

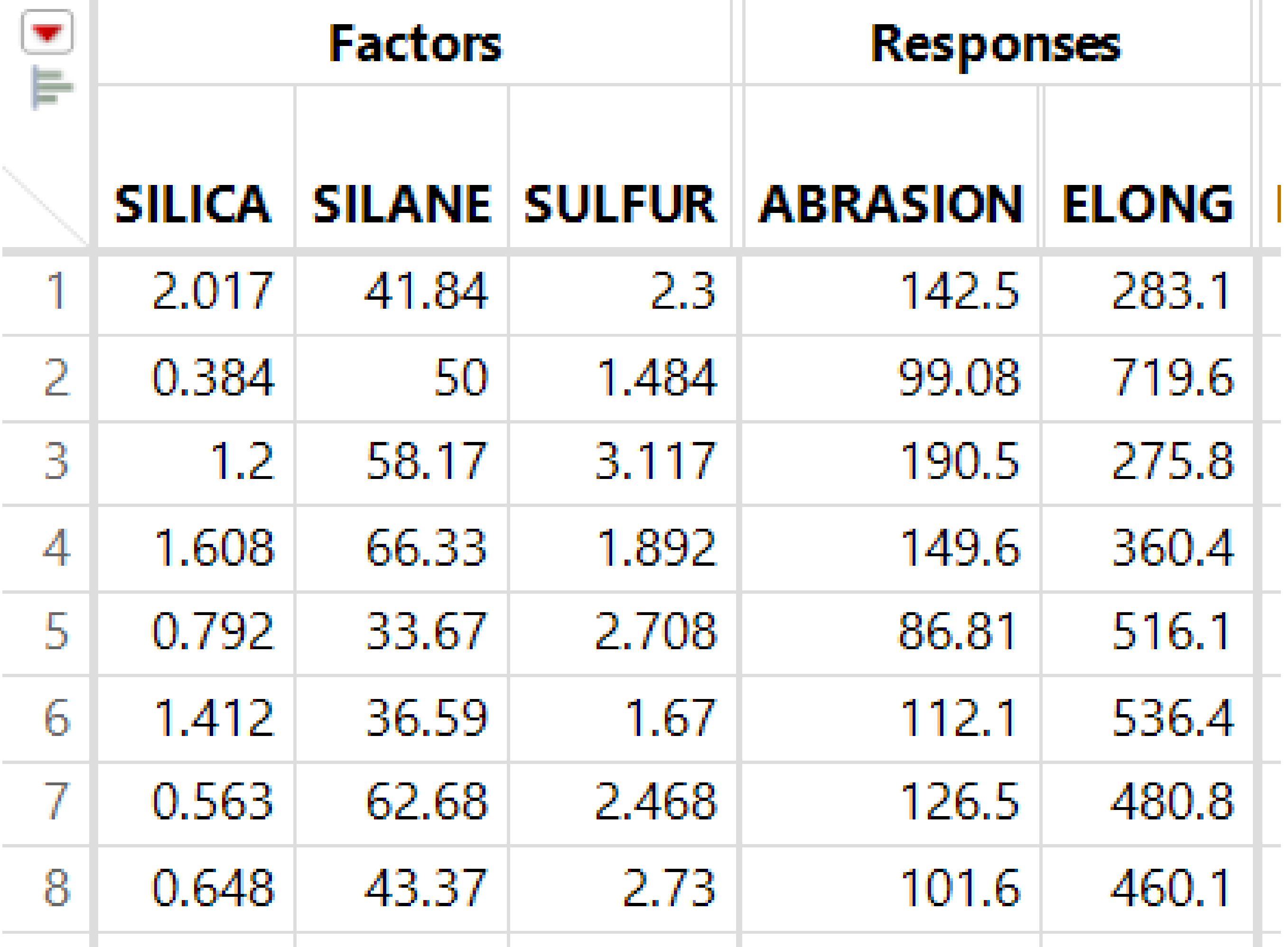
Project
Goals

=

Next Batch
Settings

Bayesian Optimization





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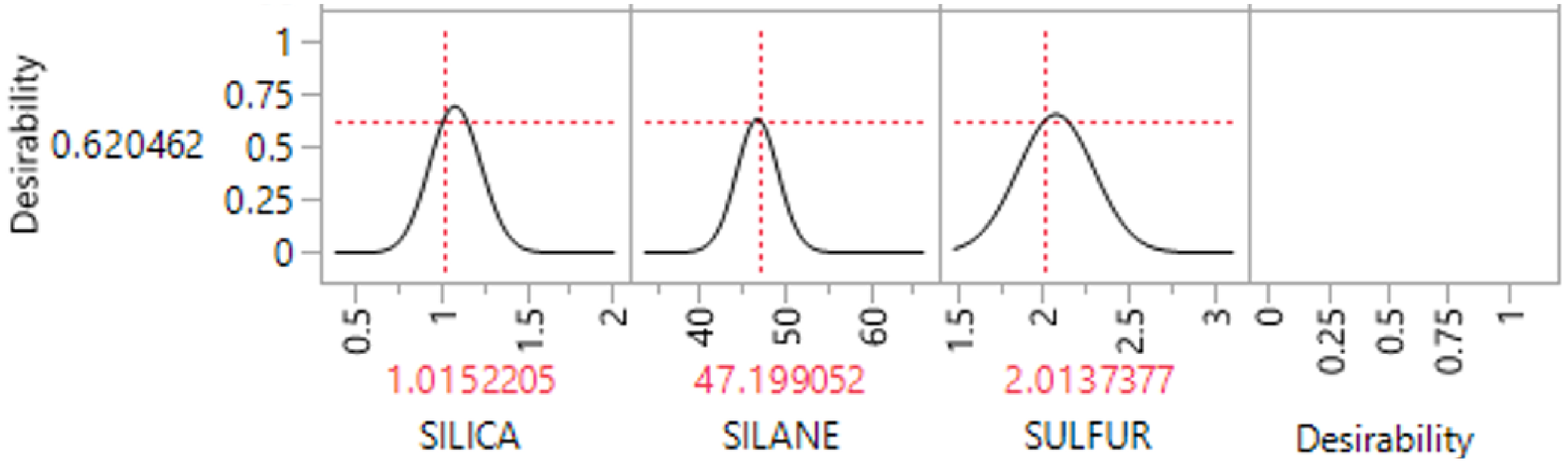
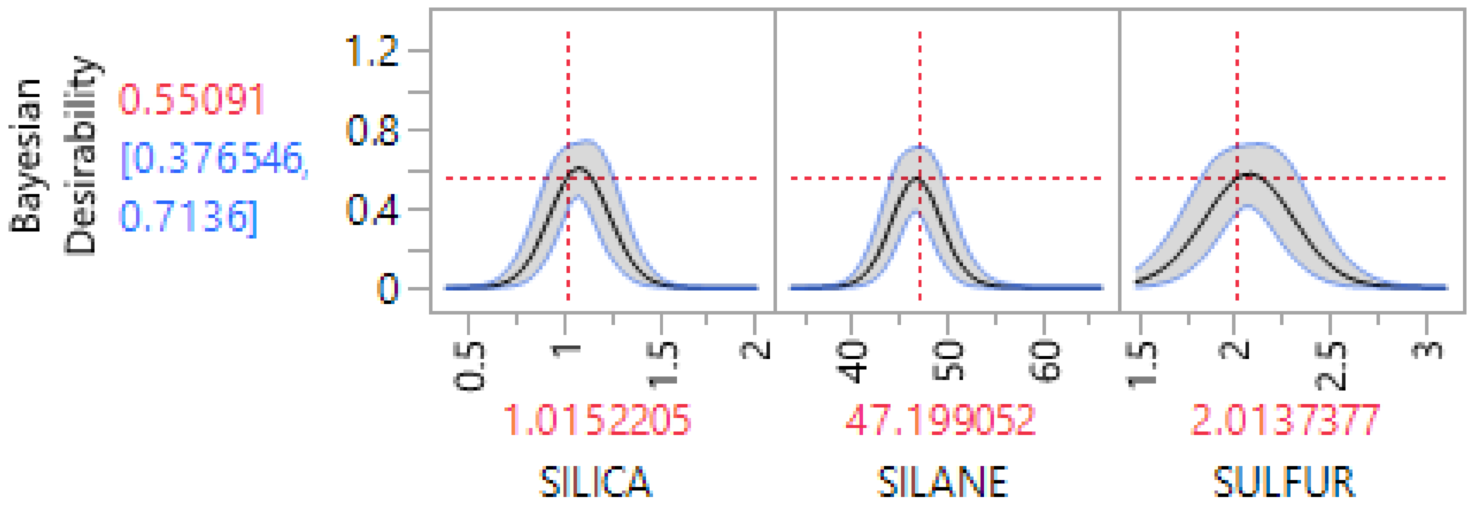
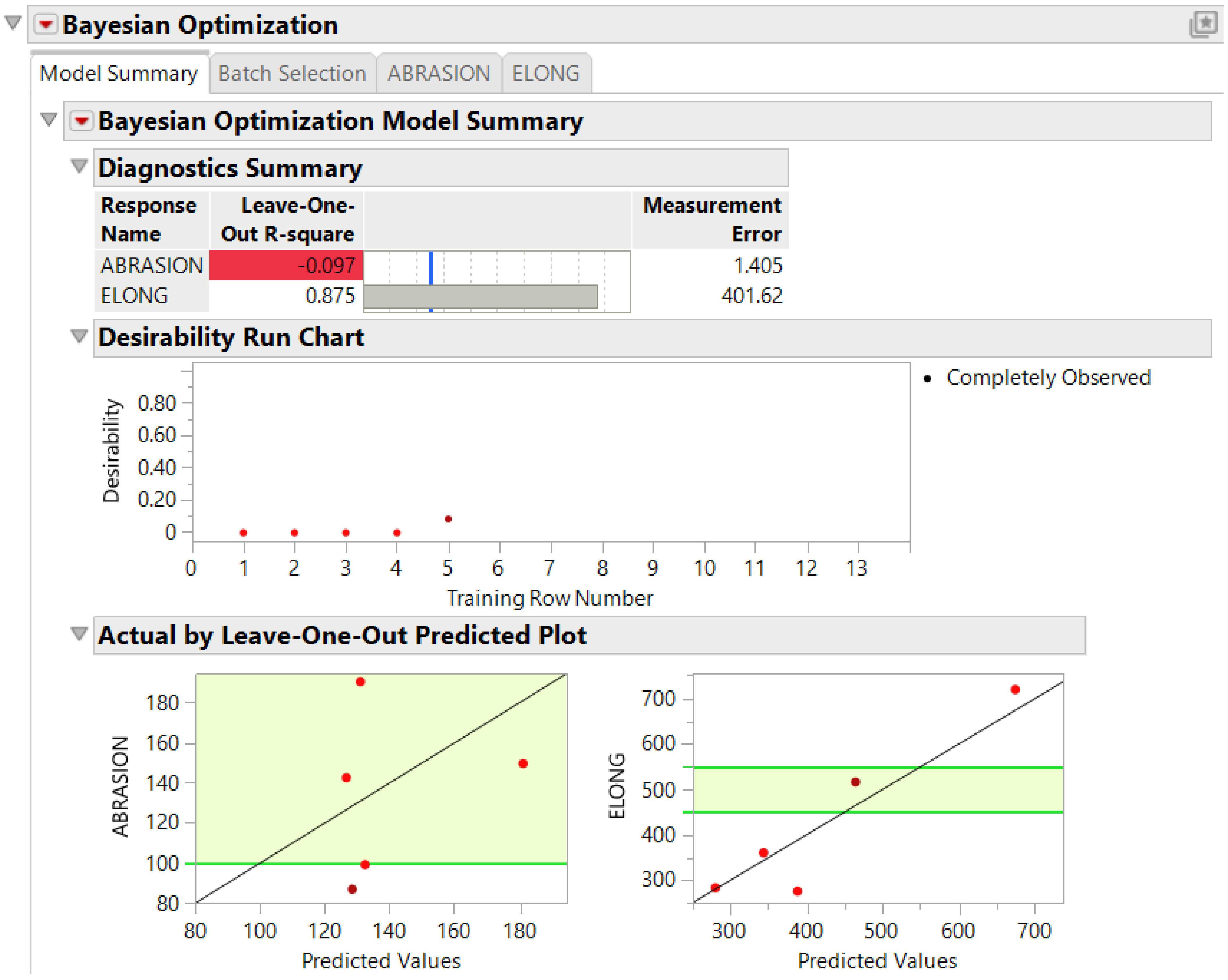
3	1.2	58.17	3.117	190.5	275.8
4	1.608	66.33	1.892	149.6	360.4
5	0.792	33.67	2.708	86.81	516.1
6	1.412	36.59	1.67	112.1	536.4
7	0.563	62.68	2.468	126.5	480.8
8	0.648	43.37	2.73	101.6	460.1





Bayesian Optimization



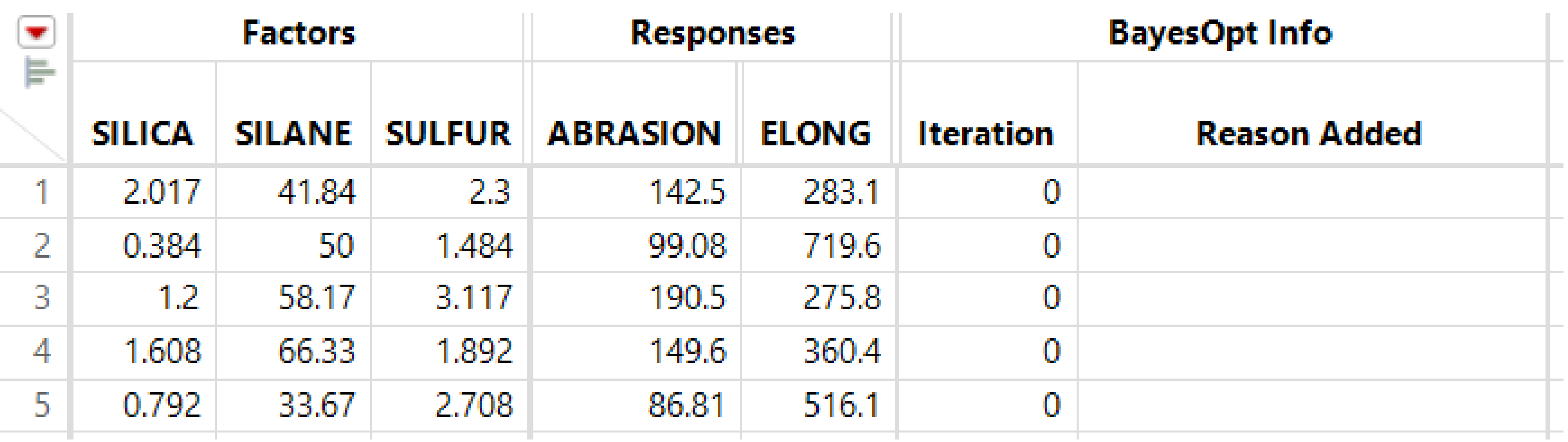
Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square	Measurement Error
ABRASION	-0.097	1.405
ELONG	0.875	401.62

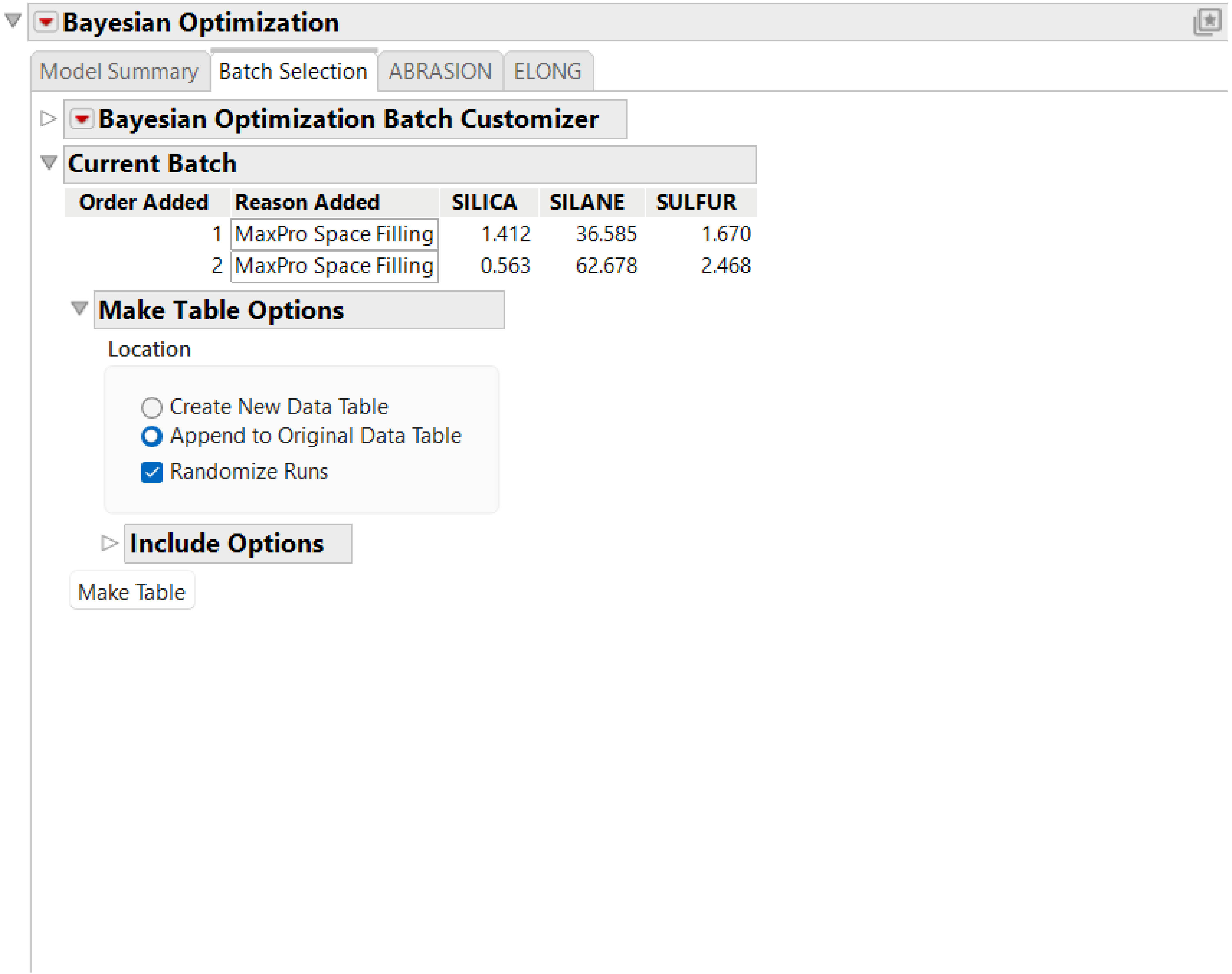
Desirability Run Chart

Actual by Leave-One-Out Predicted Plot



	Factors			Responses		BayesOpt Info	
	SILICA	SILANE	SULFUR	ABRASION	ELONG	Iteration	Reason Added
1	2.017	41.84	2.3	142.5	283.1	0	
2	0.384	50	1.484	99.08	719.6	0	
3	1.2	58.17	3.117	190.5	275.8	0	
4	1.608	66.33	1.892	149.6	360.4	0	
5	0.792	33.67	2.708	86.81	516.1	0	

Bayesian Optimization



Current Batch

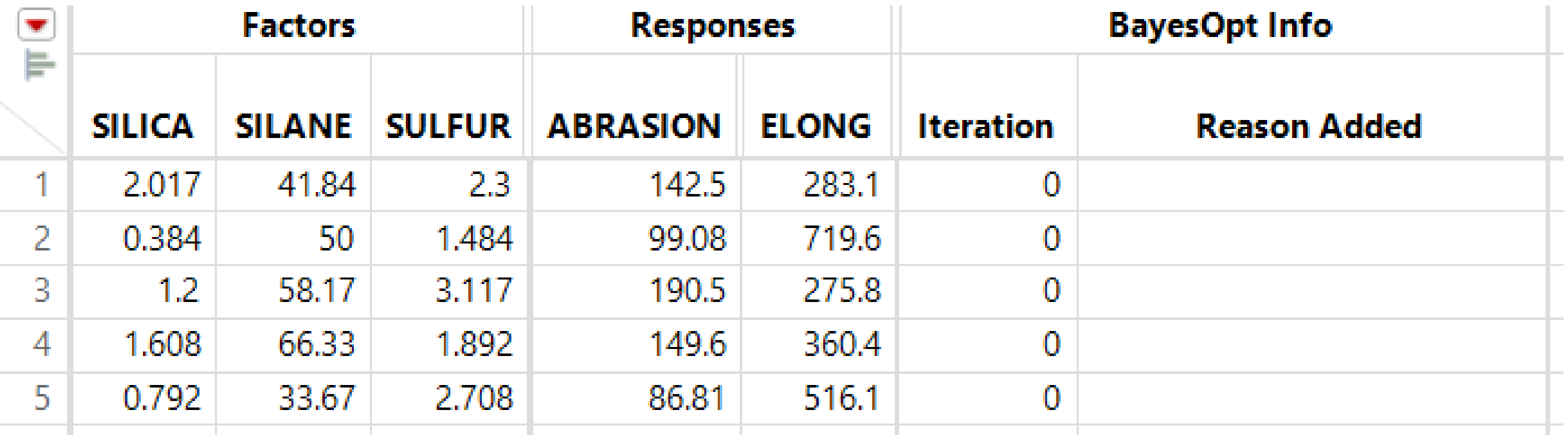
Order Added	Reason Added	SILICA	SILANE	SULFUR
1	MaxPro Space Filling	1.412	36.585	1.670
2	MaxPro Space Filling	0.563	62.678	2.468

Make Table Options

Location

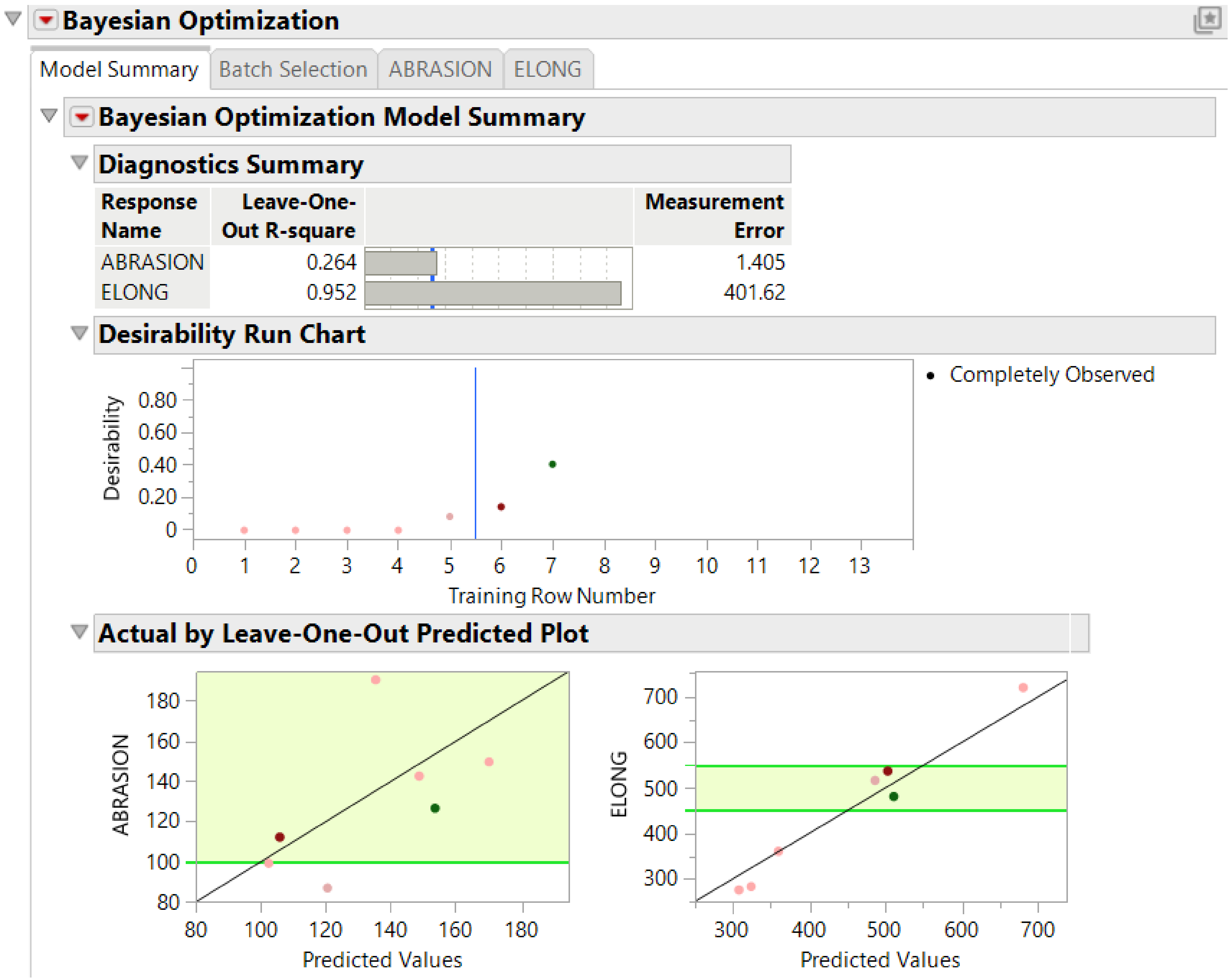
○ Create New Data Table
● Append to Original Data Table
☑ Randomize Runs

Include Options



	Factors			Responses		BayesOpt Info	
	SILICA	SILANE	SULFUR	ABRASION	ELONG	Iteration	Reason Added
1	2.017	41.84	2.3	142.5	283.1	0	
2	0.384	50	1.484	99.08	719.6	0	
3	1.2	58.17	3.117	190.5	275.8	0	
4	1.608	66.33	1.892	149.6	360.4	0	
5	0.792	33.67	2.708	86.81	516.1	0	

Bayesian Optimization



Bayesian Optimization

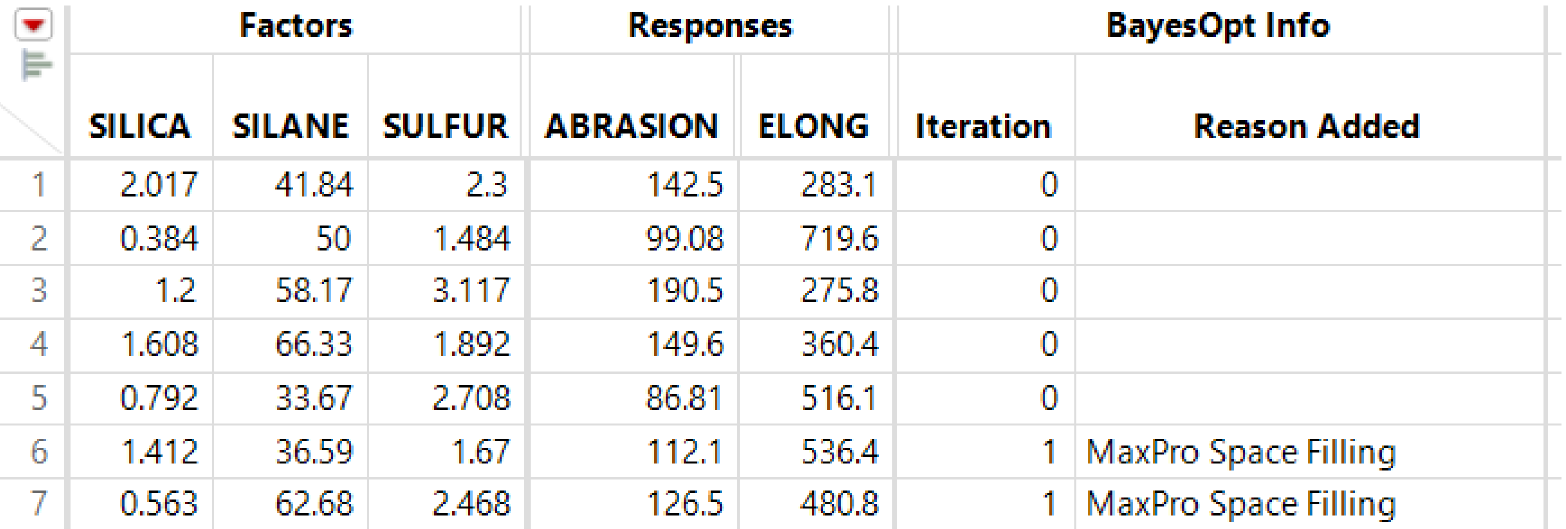
Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square	Measurement Error
ABRASION	0.264	1.405
ELONG	0.952	401.62

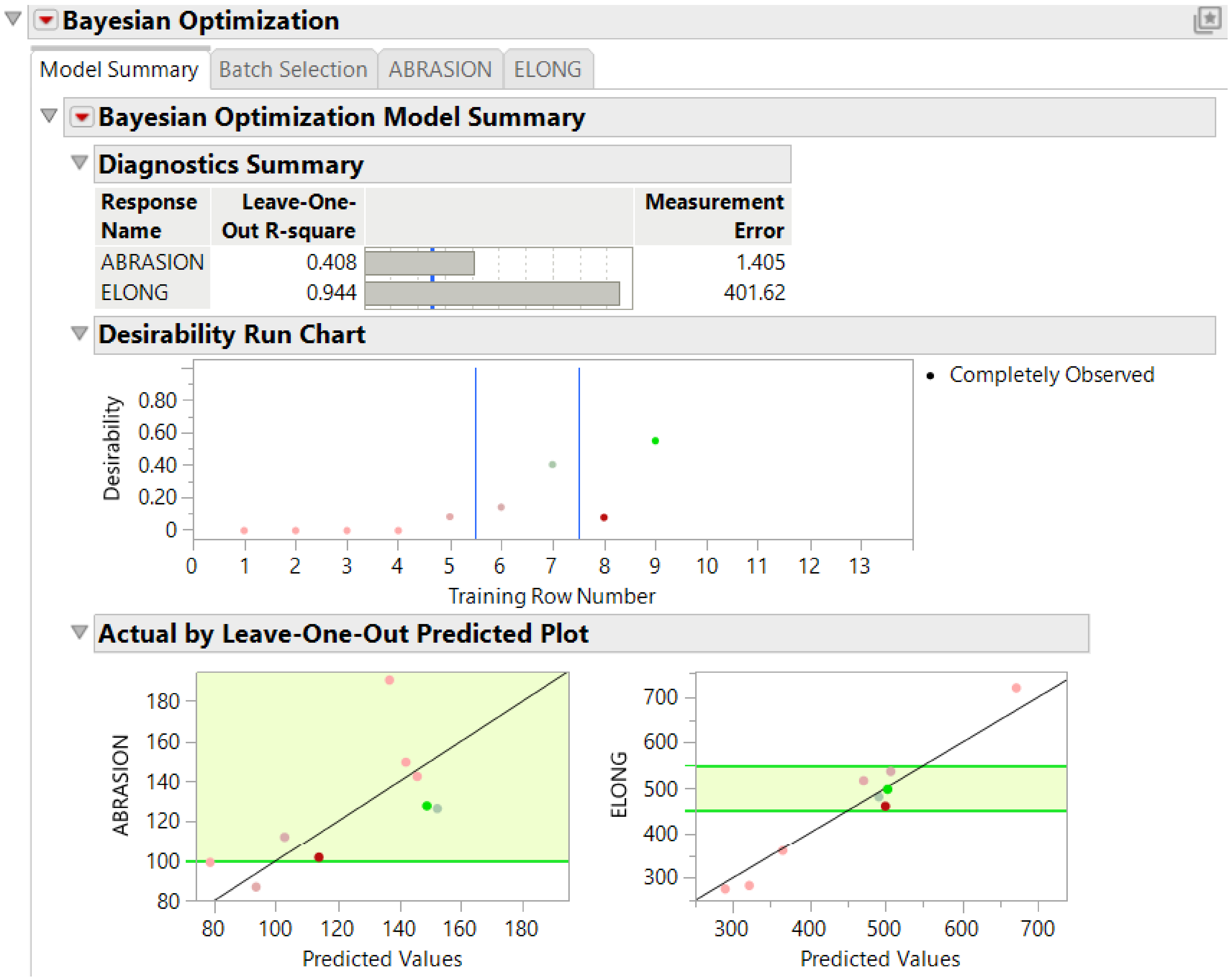
Desirability Run Chart

Actual by Leave-One-Out Predicted Plot



	Factors			Responses		BayesOpt Info	
	SILICA	SILANE	SULFUR	ABRASION	ELONG	Iteration	Reason Added
1	2.017	41.84	2.3	142.5	283.1	0	
2	0.384	50	1.484	99.08	719.6	0	
3	1.2	58.17	3.117	190.5	275.8	0	
4	1.608	66.33	1.892	149.6	360.4	0	
5	0.792	33.67	2.708	86.81	516.1	0	
6	1.412	36.59	1.67	112.1	536.4	1	MaxPro Space Filling
7	0.563	62.68	2.468	126.5	480.8	1	MaxPro Space Filling

Bayesian Optimization



Bayesian Optimization

Model Summary | Batch Selection | ABRASION | ELONG

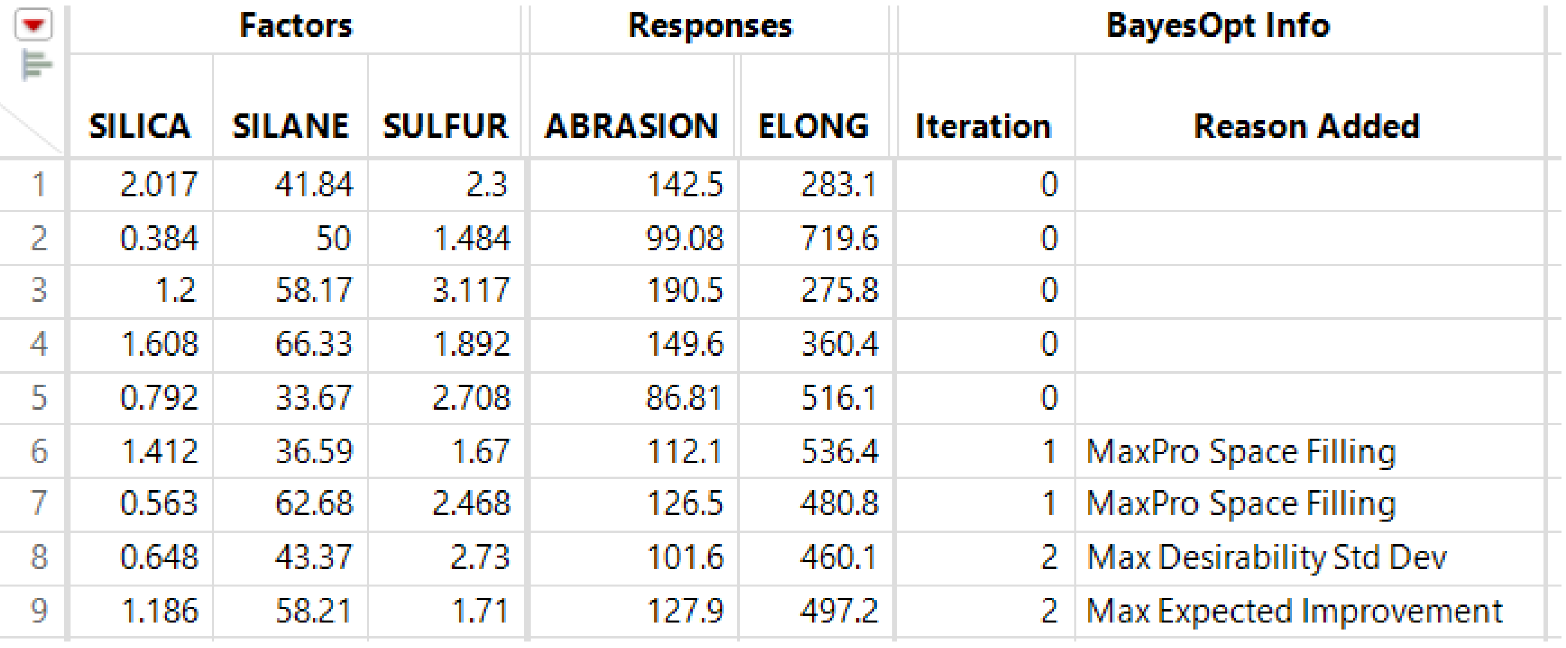
Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square		Measurement Error
ABRASION	0.408		1.405
ELONG	0.944		401.62

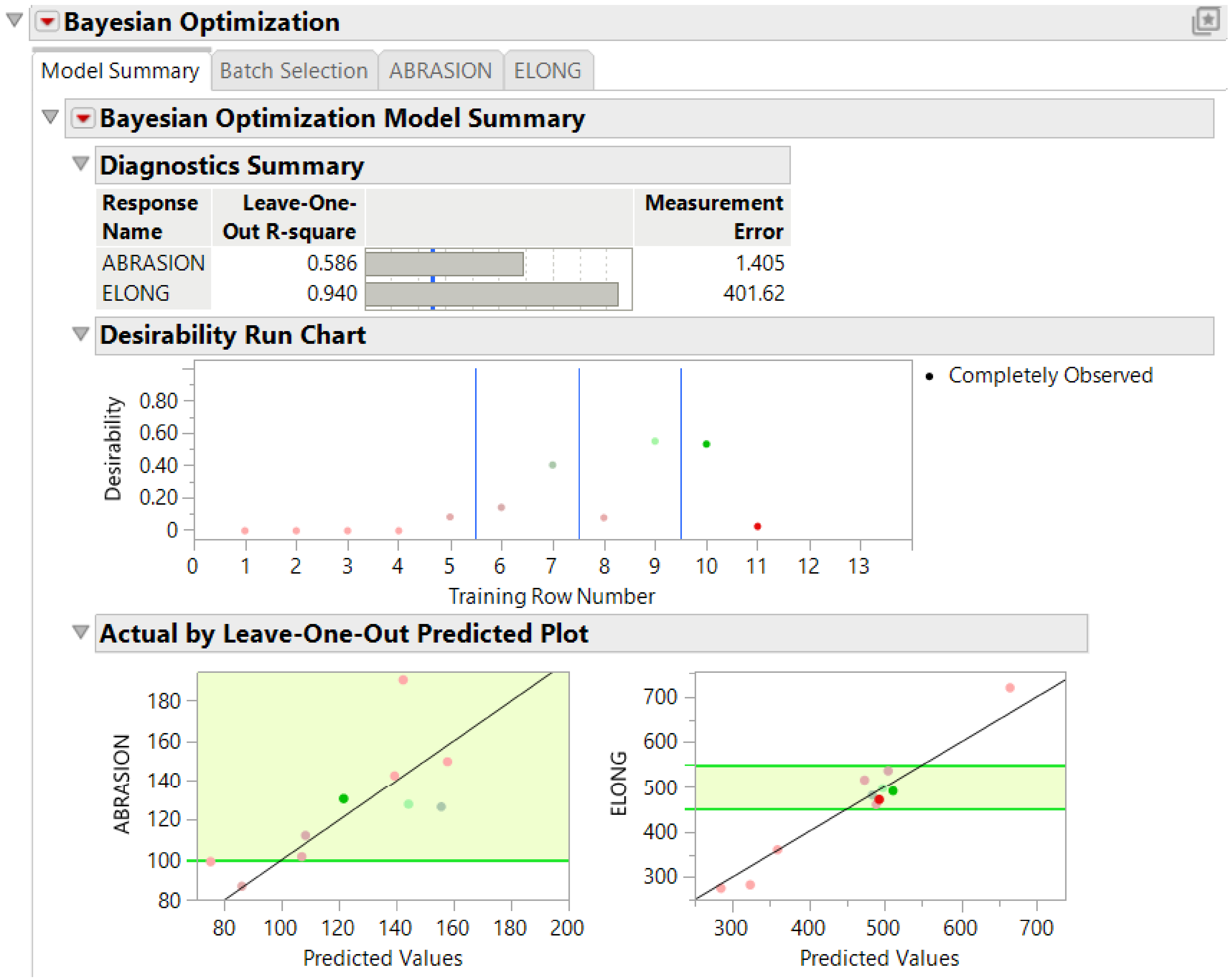
Desirability Run Chart

Actual by Leave-One-Out Predicted Plot



	Factors			Responses		BayesOpt Info	
	SILICA	**SILANE**	**SULFUR**	**ABRASION**	**ELONG**	**Iteration**	**Reason Added**
1	2.017	41.84	2.3	142.5	283.1	0	
2	0.384	50	1.484	99.08	719.6	0	
3	1.2	58.17	3.117	190.5	275.8	0	
4	1.608	66.33	1.892	149.6	360.4	0	
5	0.792	33.67	2.708	86.81	516.1	0	
6	1.412	36.59	1.67	112.1	536.4	1	MaxPro Space Filling
7	0.563	62.68	2.468	126.5	480.8	1	MaxPro Space Filling
8	0.648	43.37	2.73	101.6	460.1	2	Max Desirability Std Dev
9	1.186	58.21	1.71	127.9	497.2	2	Max Expected Improvement

Bayesian Optimization



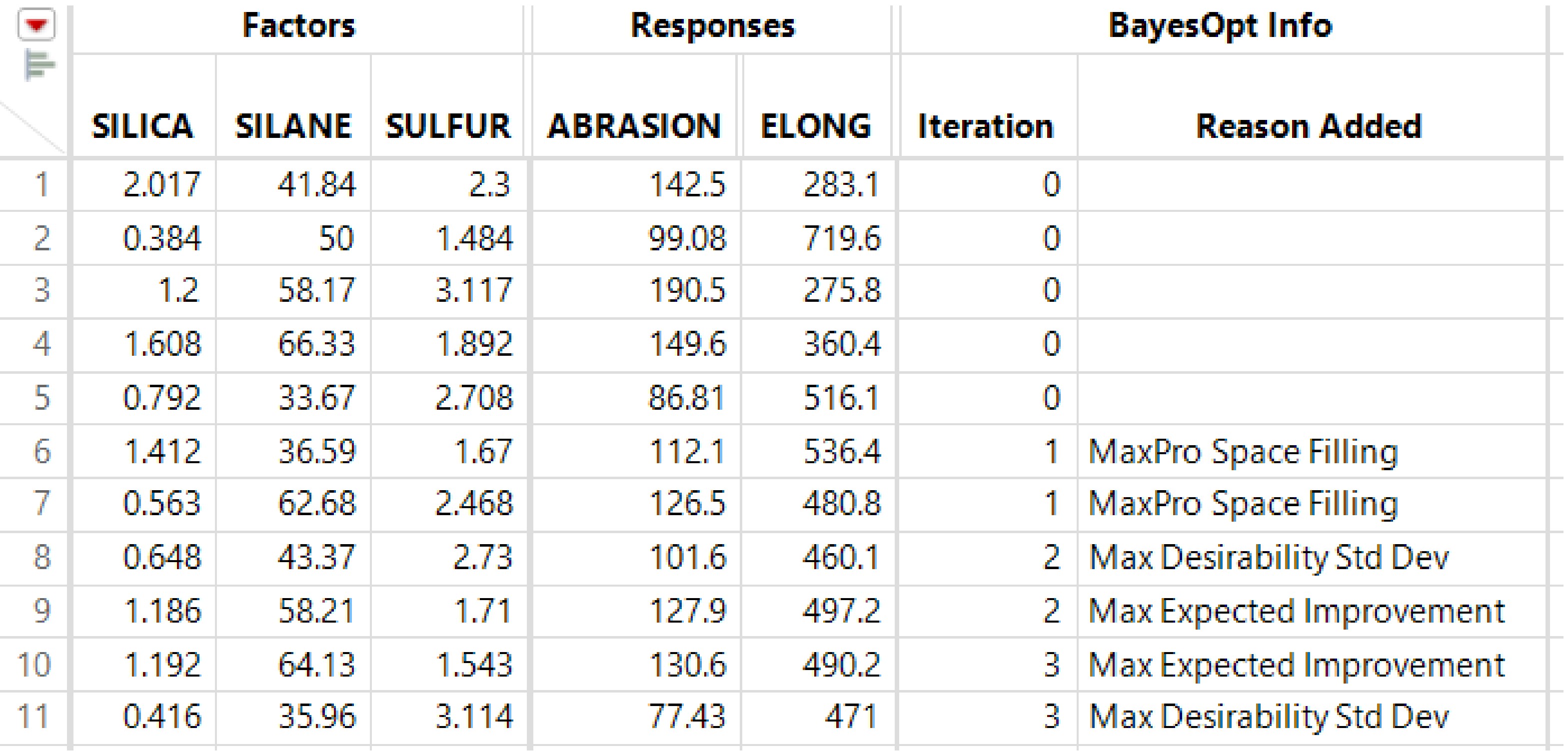
Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square	Measurement Error
ABRASION	0.586	1.405
ELONG	0.940	401.62

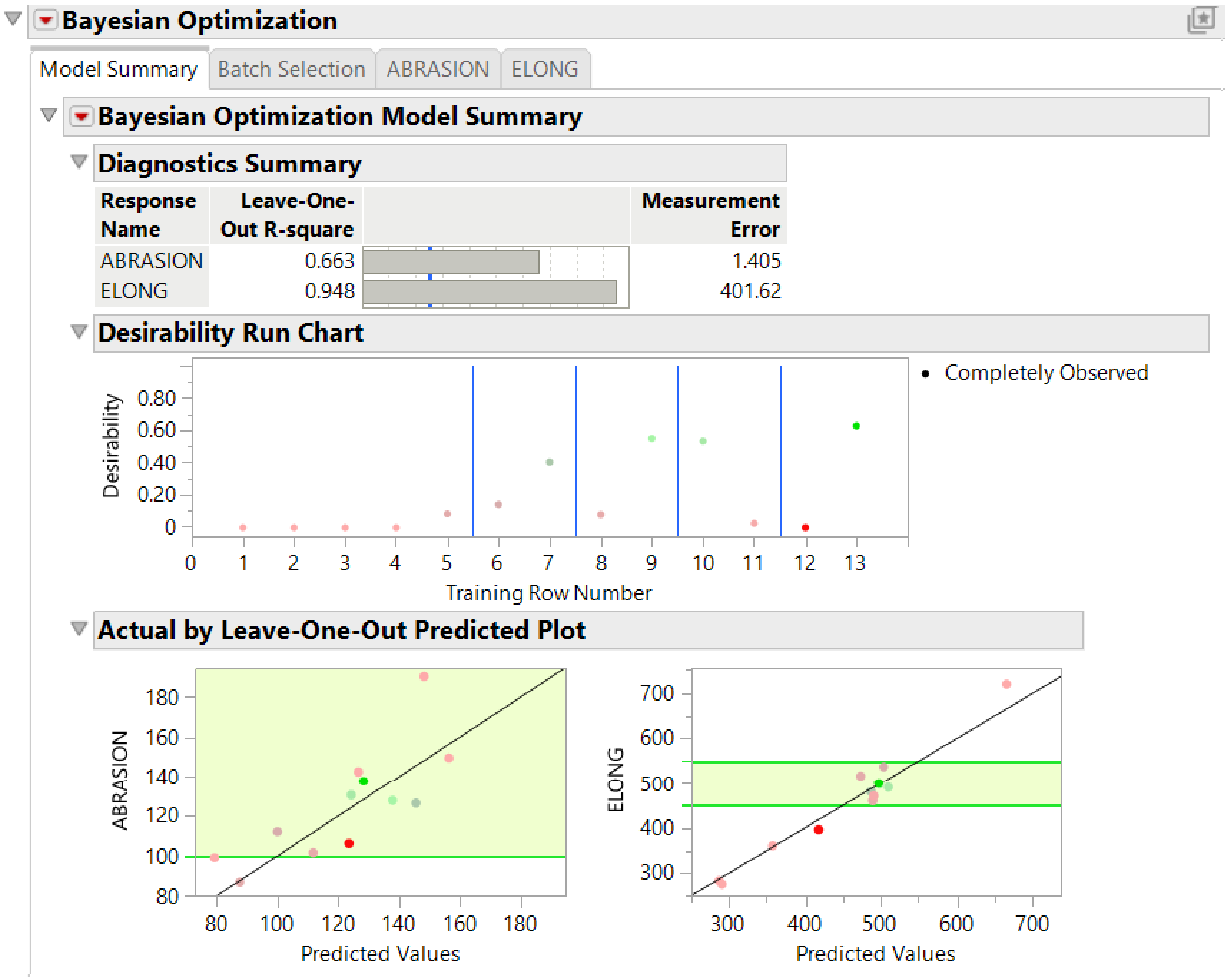
Desirability Run Chart

Actual by Leave-One-Out Predicted Plot



	Factors			Responses		BayesOpt Info	
	SILICA	**SILANE**	**SULFUR**	**ABRASION**	**ELONG**	**Iteration**	**Reason Added**
1	2.017	41.84	2.3	142.5	283.1	0	
2	0.384	50	1.484	99.08	719.6	0	
3	1.2	58.17	3.117	190.5	275.8	0	
4	1.608	66.33	1.892	149.6	360.4	0	
5	0.792	33.67	2.708	86.81	516.1	0	
6	1.412	36.59	1.67	112.1	536.4	1	MaxPro Space Filling
7	0.563	62.68	2.468	126.5	480.8	1	MaxPro Space Filling
8	0.648	43.37	2.73	101.6	460.1	2	Max Desirability Std Dev
9	1.186	58.21	1.71	127.9	497.2	2	Max Expected Improvement
10	1.192	64.13	1.543	130.6	490.2	3	Max Expected Improvement
11	0.416	35.96	3.114	77.43	471	3	Max Desirability Std Dev

Bayesian Optimization



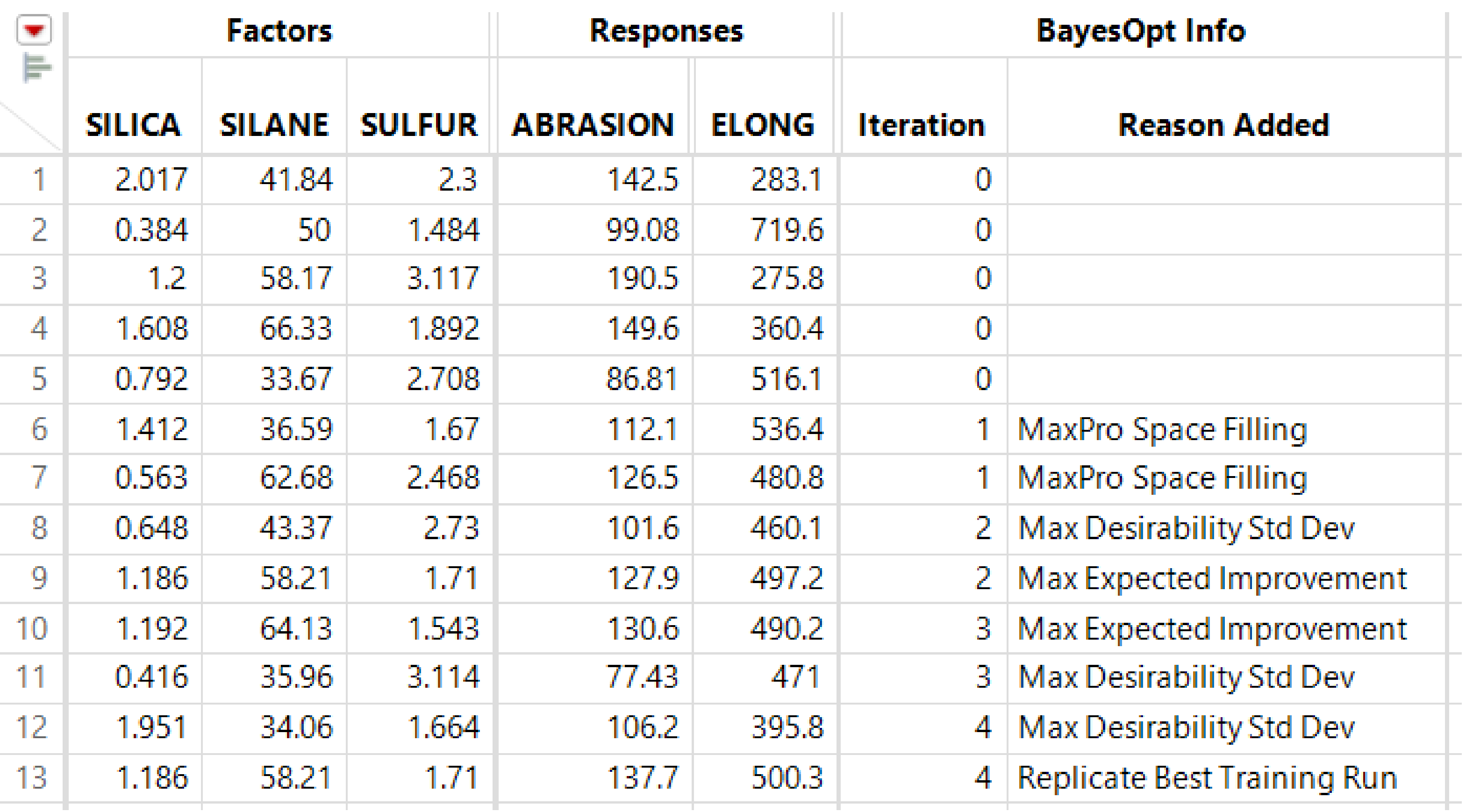
Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square		Measurement Error
ABRASION	0.663		1.405
ELONG	0.948		401.62

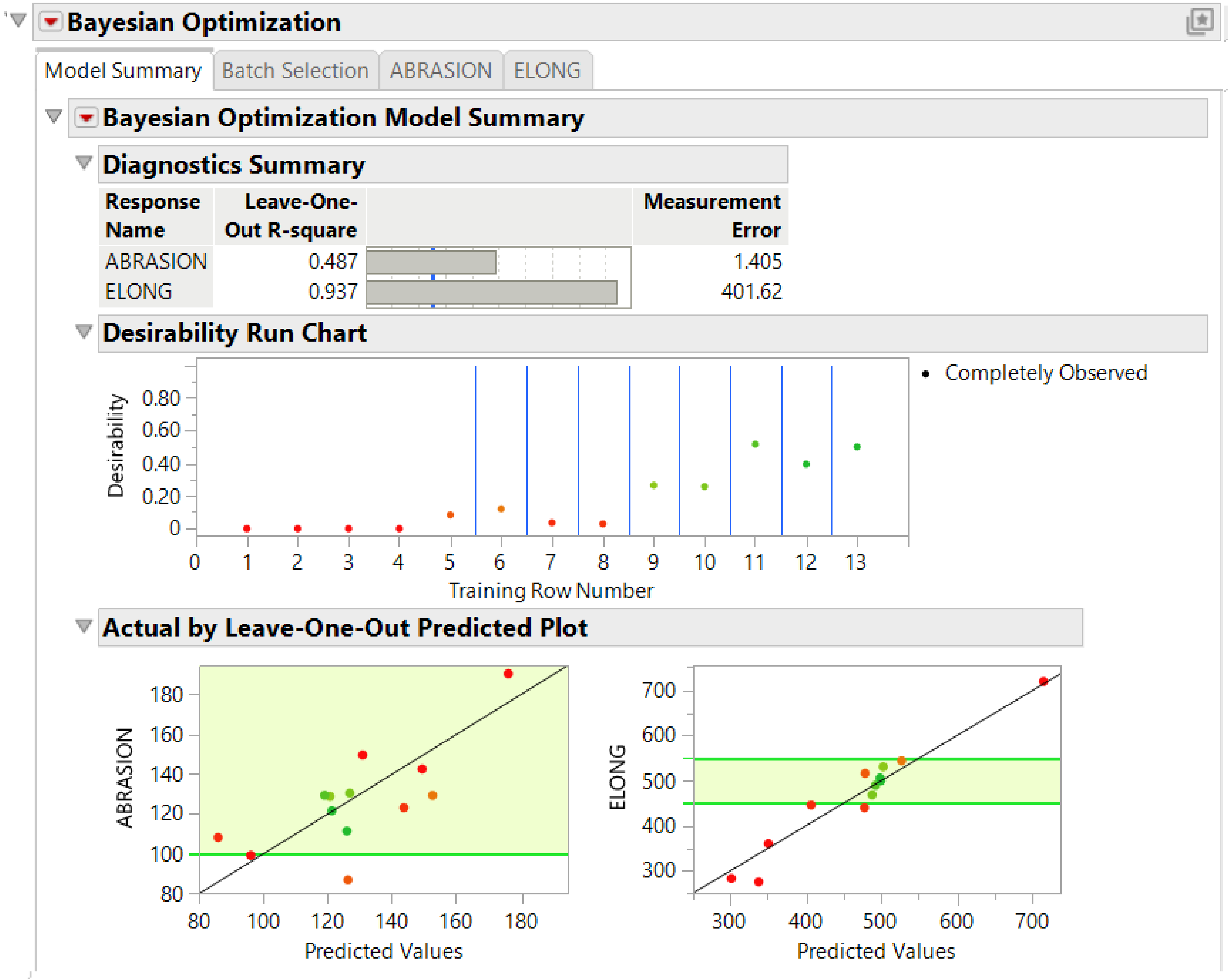
Desirability Run Chart

Actual by Leave-One-Out Predicted Plot



	Factors			Responses		BayesOpt Info	
	SILICA	SILANE	SULFUR	ABRASION	ELONG	Iteration	Reason Added
1	2.017	41.84	2.3	142.5	283.1	0	
2	0.384	50	1.484	99.08	719.6	0	
3	1.2	58.17	3.117	190.5	275.8	0	
4	1.608	66.33	1.892	149.6	360.4	0	
5	0.792	33.67	2.708	86.81	516.1	0	
6	1.412	36.59	1.67	112.1	536.4	1	MaxPro Space Filling
7	0.563	62.68	2.468	126.5	480.8	1	MaxPro Space Filling
8	0.648	43.37	2.73	101.6	460.1	2	Max Desirability Std Dev
9	1.186	58.21	1.71	127.9	497.2	2	Max Expected Improvement
10	1.192	64.13	1.543	130.6	490.2	3	Max Expected Improvement
11	0.416	35.96	3.114	77.43	471	3	Max Desirability Std Dev
12	1.951	34.06	1.664	106.2	395.8	4	Max Desirability Std Dev
13	1.186	58.21	1.71	137.7	500.3	4	Replicate Best Training Run

Bayesian Optimization



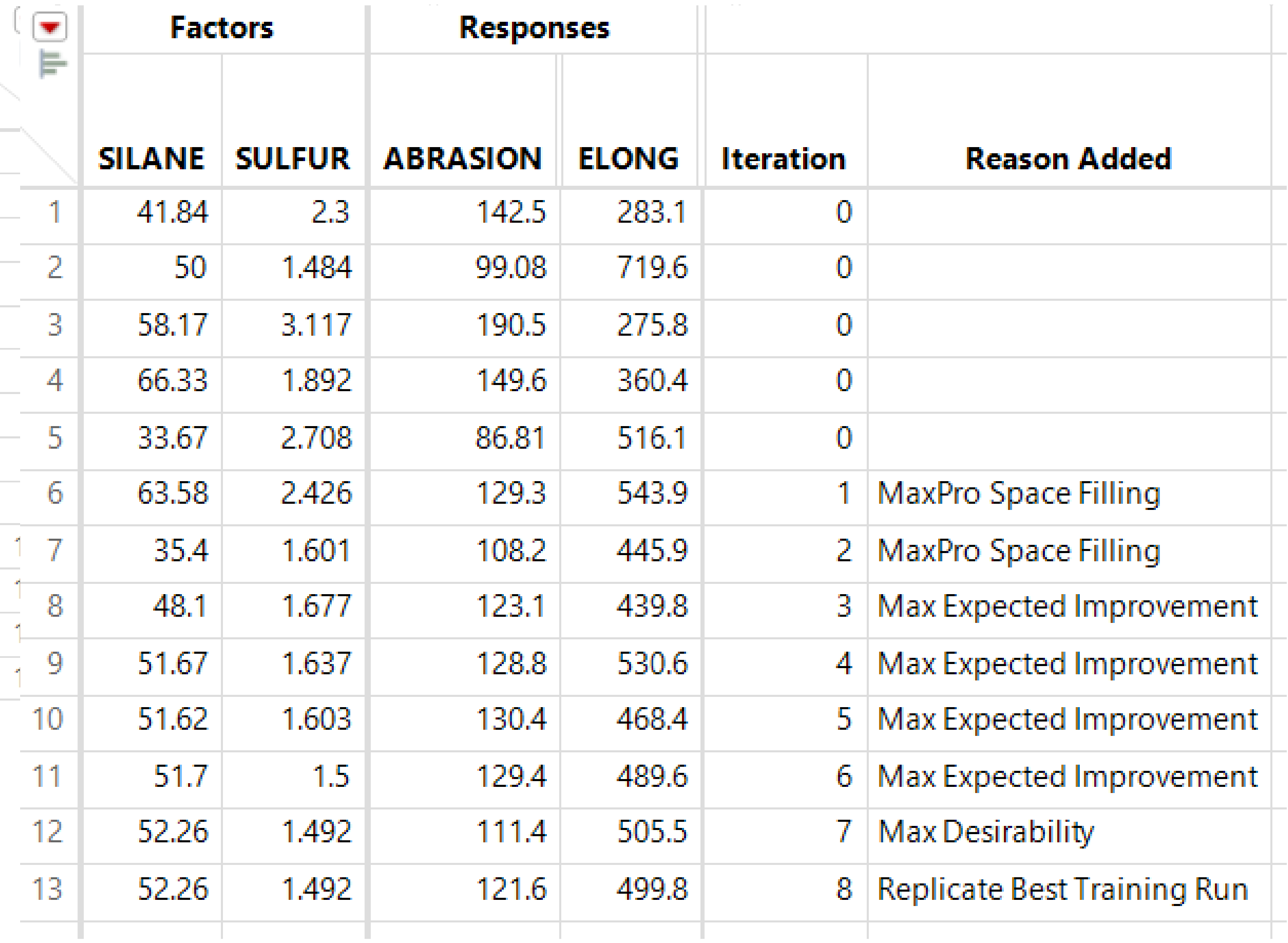
Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square		Measurement Error
ABRASION	0.487		1.405
ELONG	0.937		401.62

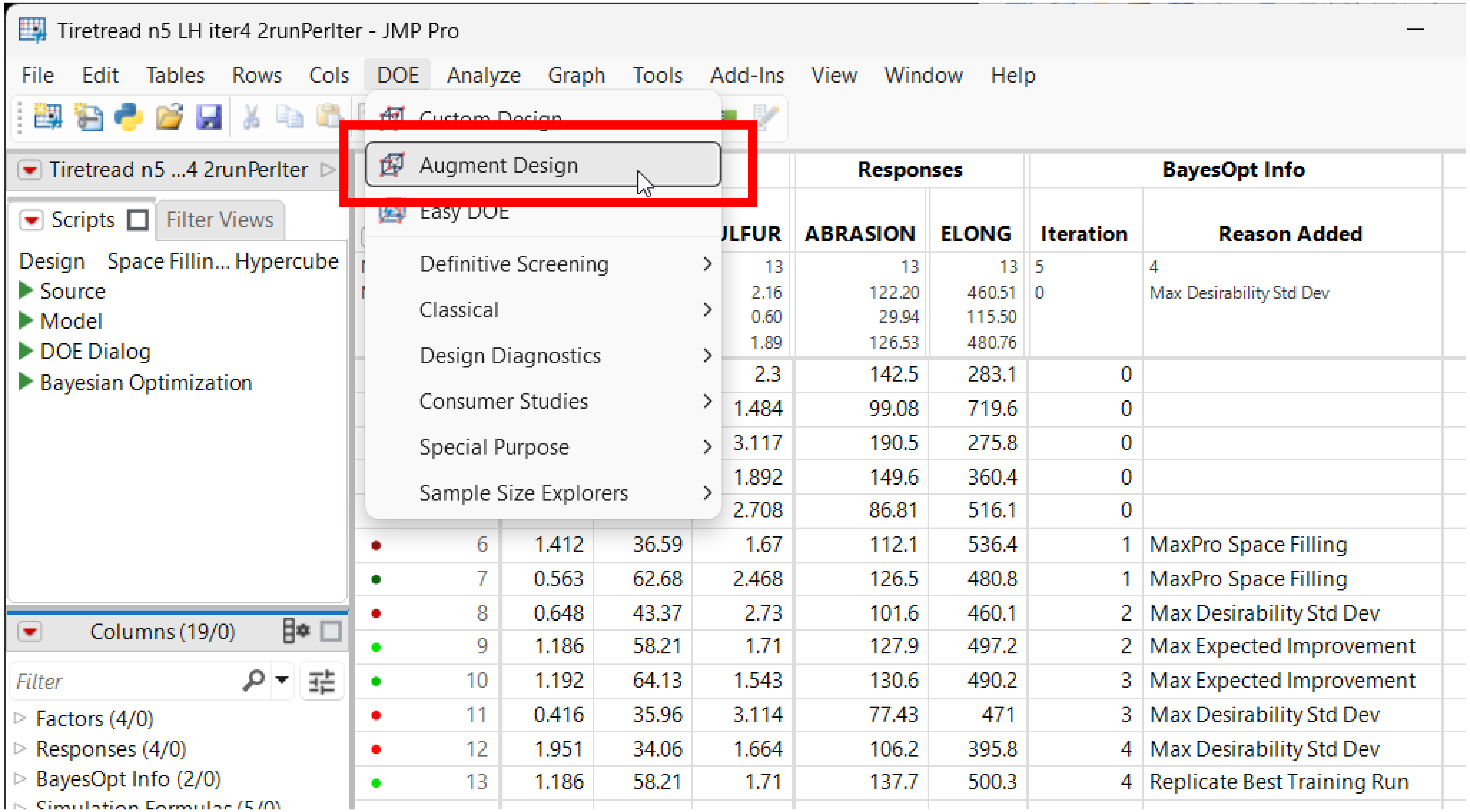
Desirability Run Chart

Actual by Leave-One-Out Predicted Plot



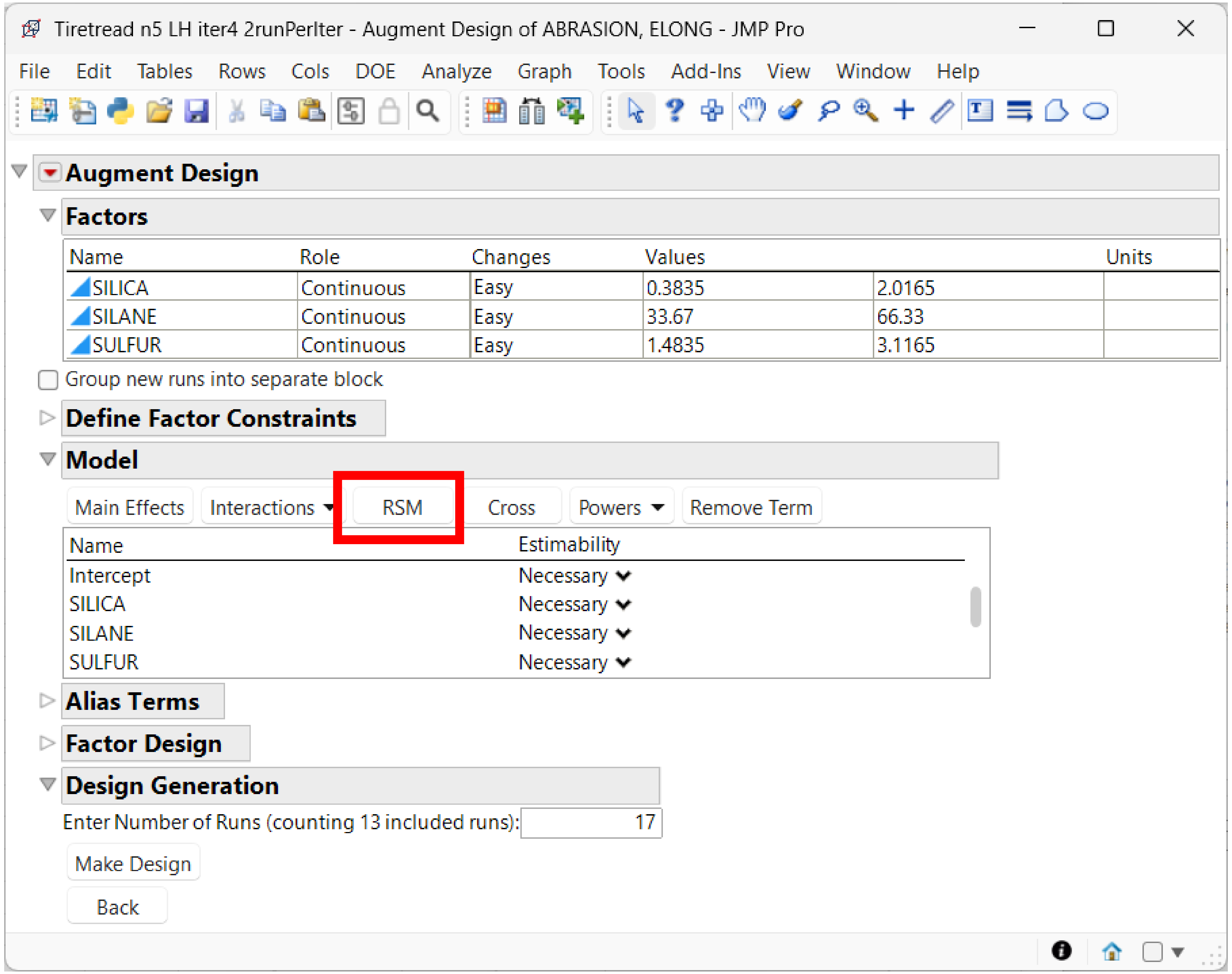
	Factors		Responses			
	SILANE	SULFUR	ABRASION	ELONG	Iteration	Reason Added
1	41.84	2.3	142.5	283.1	0	
2	50	1.484	99.08	719.6	0	
3	58.17	3.117	190.5	275.8	0	
4	66.33	1.892	149.6	360.4	0	
5	33.67	2.708	86.81	516.1	0	
6	63.58	2.426	129.3	543.9	1	MaxPro Space Filling
7	35.4	1.601	108.2	445.9	2	MaxPro Space Filling
8	48.1	1.677	123.1	439.8	3	Max Expected Improvement
9	51.67	1.637	128.8	530.6	4	Max Expected Improvement
10	51.62	1.603	130.4	468.4	5	Max Expected Improvement
11	51.7	1.5	129.4	489.6	6	Max Expected Improvement
12	52.26	1.492	111.4	505.5	7	Max Desirability
13	52.26	1.492	121.6	499.8	8	Replicate Best Training Run

Bayesian Optimization



					Responses		BayesOpt Info	
				ULFUR	ABRASION	ELONG	Iteration	Reason Added
				13 2.16 0.60 1.89	13 122.20 29.94 126.53	13 460.51 115.50 480.76	5 0	4 Max Desirability Std Dev
				2.3	142.5	283.1	0	
				1.484	99.08	719.6	0	
				3.117	190.5	275.8	0	
				1.892	149.6	360.4	0	
				2.708	86.81	516.1	0	
●	6	1.412	36.59	1.67	112.1	536.4	1	MaxPro Space Filling
●	7	0.563	62.68	2.468	126.5	480.8	1	MaxPro Space Filling
●	8	0.648	43.37	2.73	101.6	460.1	2	Max Desirability Std Dev
●	9	1.186	58.21	1.71	127.9	497.2	2	Max Expected Improvement
●	10	1.192	64.13	1.543	130.6	490.2	3	Max Expected Improvement
●	11	0.416	35.96	3.114	77.43	471	3	Max Desirability Std Dev
●	12	1.951	34.06	1.664	106.2	395.8	4	Max Desirability Std Dev
●	13	1.186	58.21	1.71	137.7	500.3	4	Replicate Best Training Run

Bayesian Optimization



Factors

Name	Role	Changes	Values		Units
SILICA	Continuous	Easy	0.3835	2.0165	
SILANE	Continuous	Easy	33.67	66.33	
SULFUR	Continuous	Easy	1.4835	3.1165	

☐ Group new runs into separate block

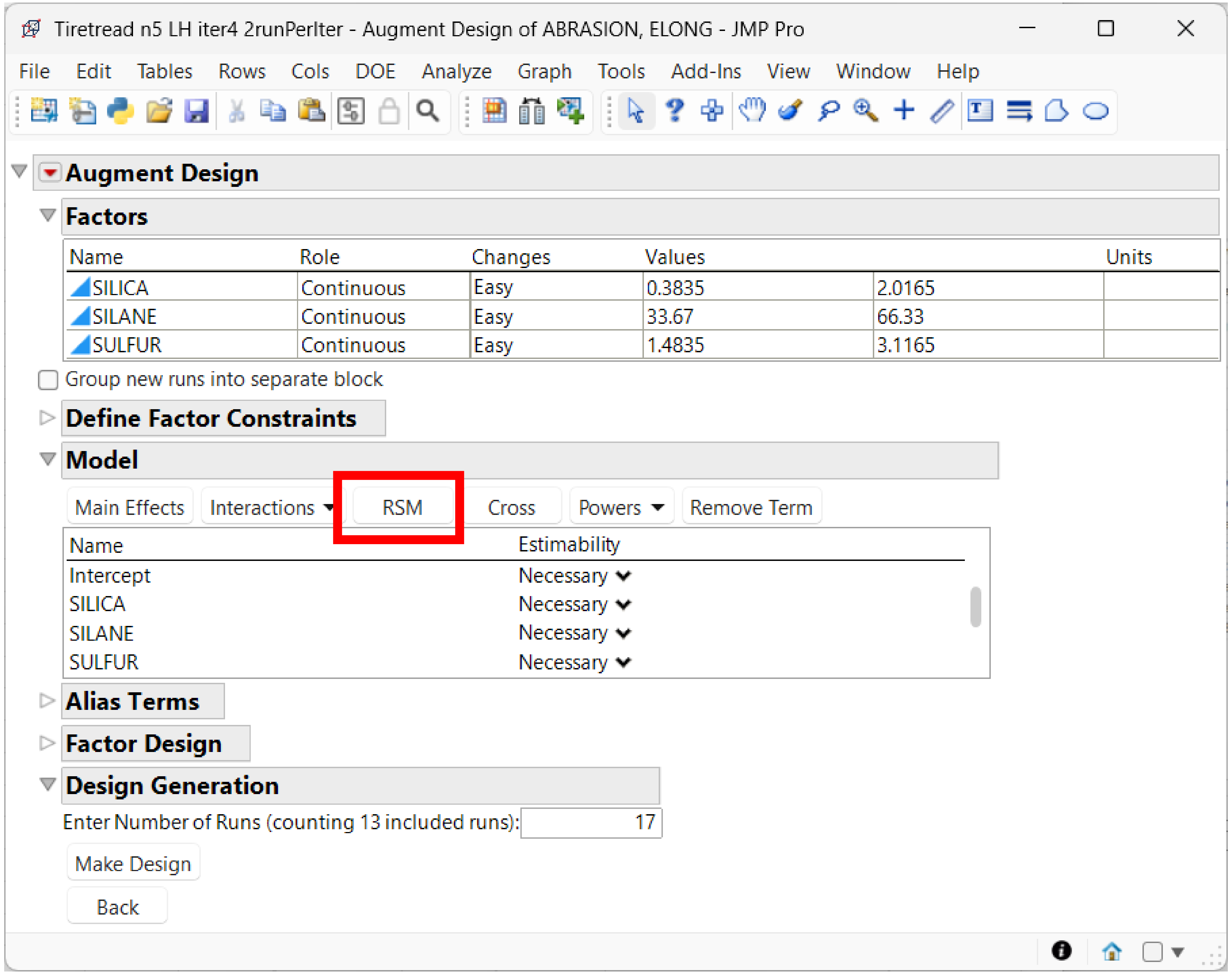
Model

Name	Estimability
Intercept	Necessary
SILICA	Necessary
SILANE	Necessary
SULFUR	Necessary

Design Generation

Enter Number of Runs (counting 13 included runs): 17

Bayesian Optimization



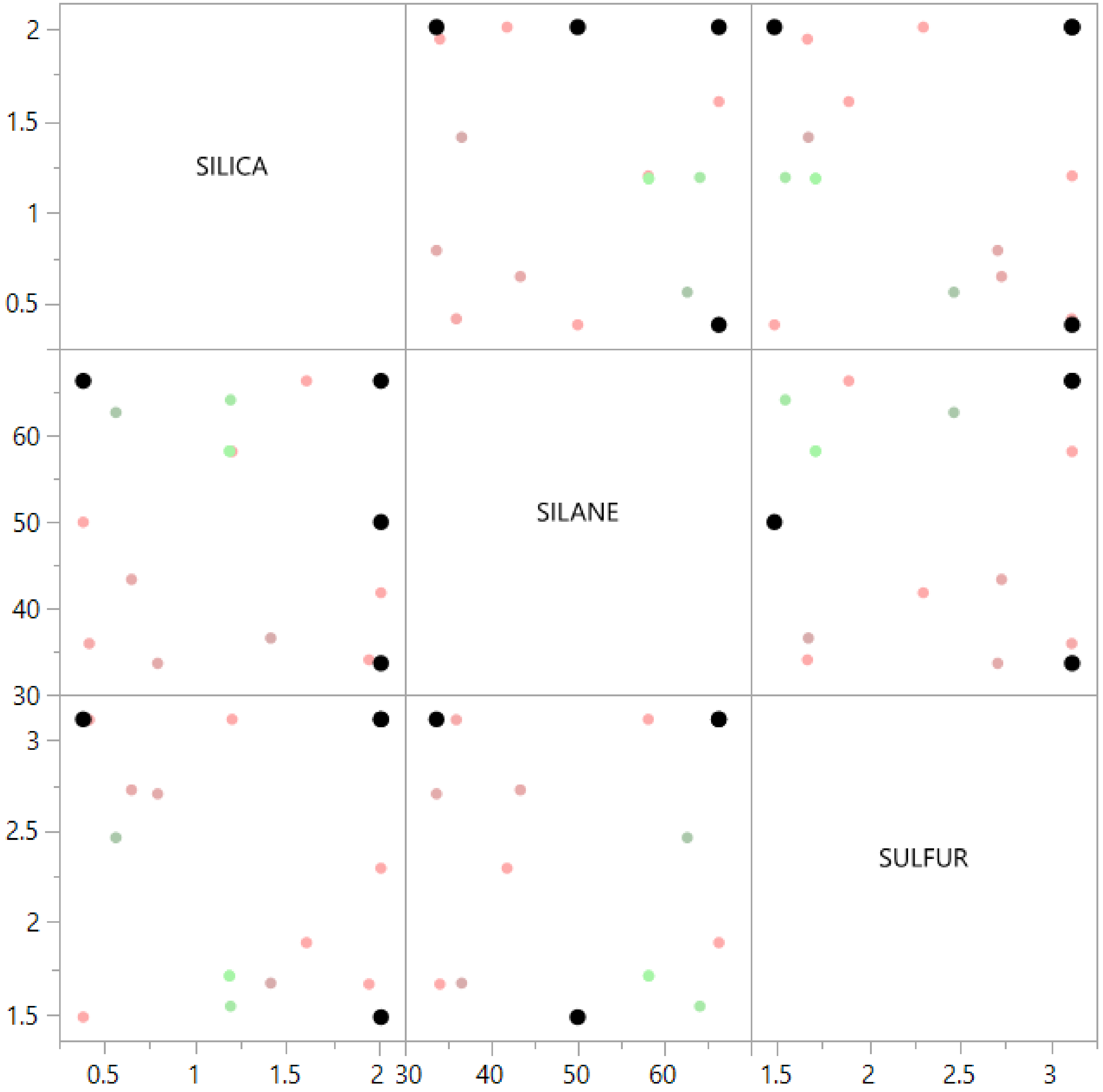
Name	Role	Changes	Values		Units
SILICA	Continuous	Easy	0.3835	2.0165	
SILANE	Continuous	Easy	33.67	66.33	
SULFUR	Continuous	Easy	1.4835	3.1165	

☐ Group new runs into separate block

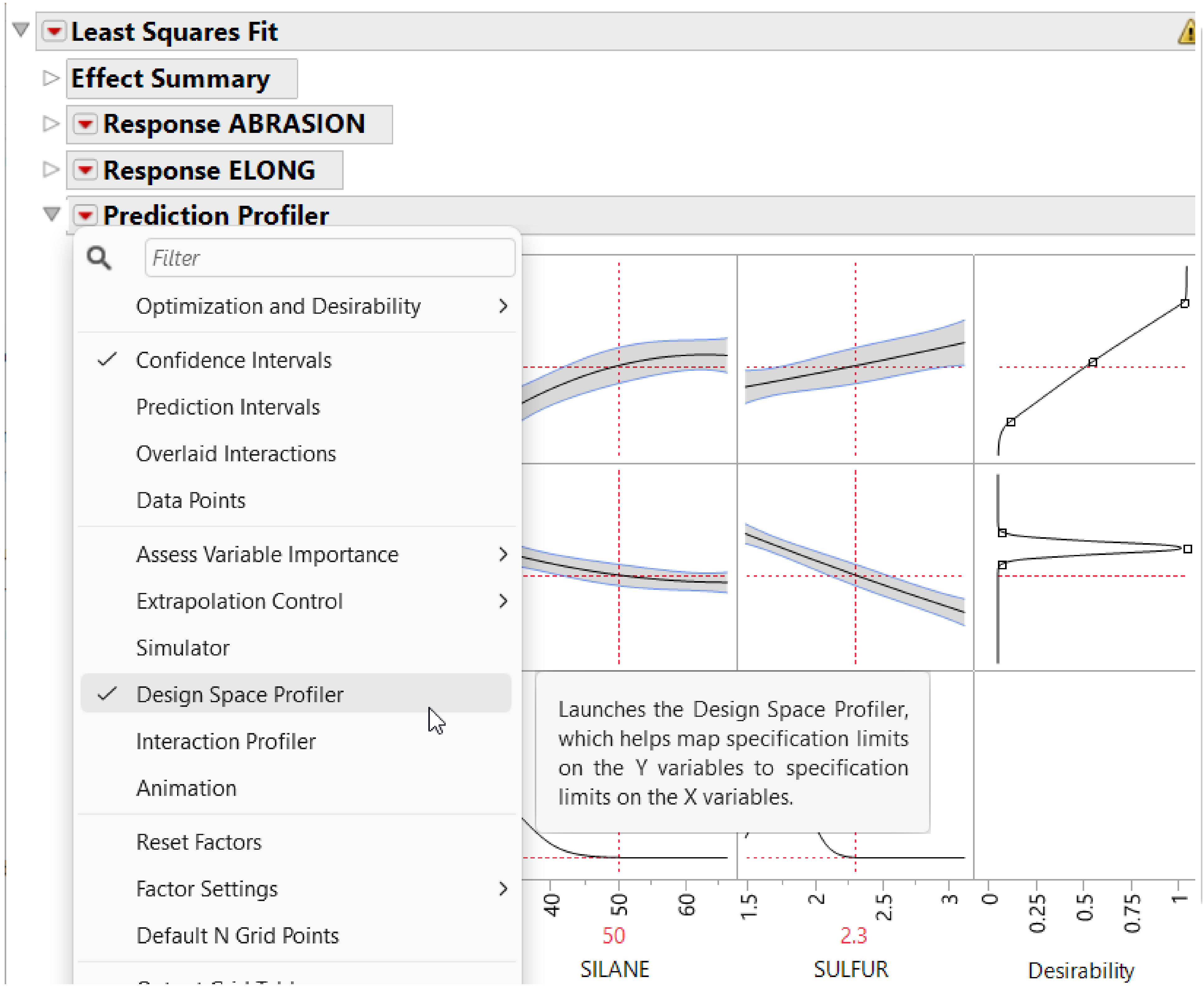
Name	Estimability
Intercept	Necessary
SILICA	Necessary
SILANE	Necessary
SULFUR	Necessary

Enter Number of Runs (counting 13 included runs): 17

Bayesian Optimization

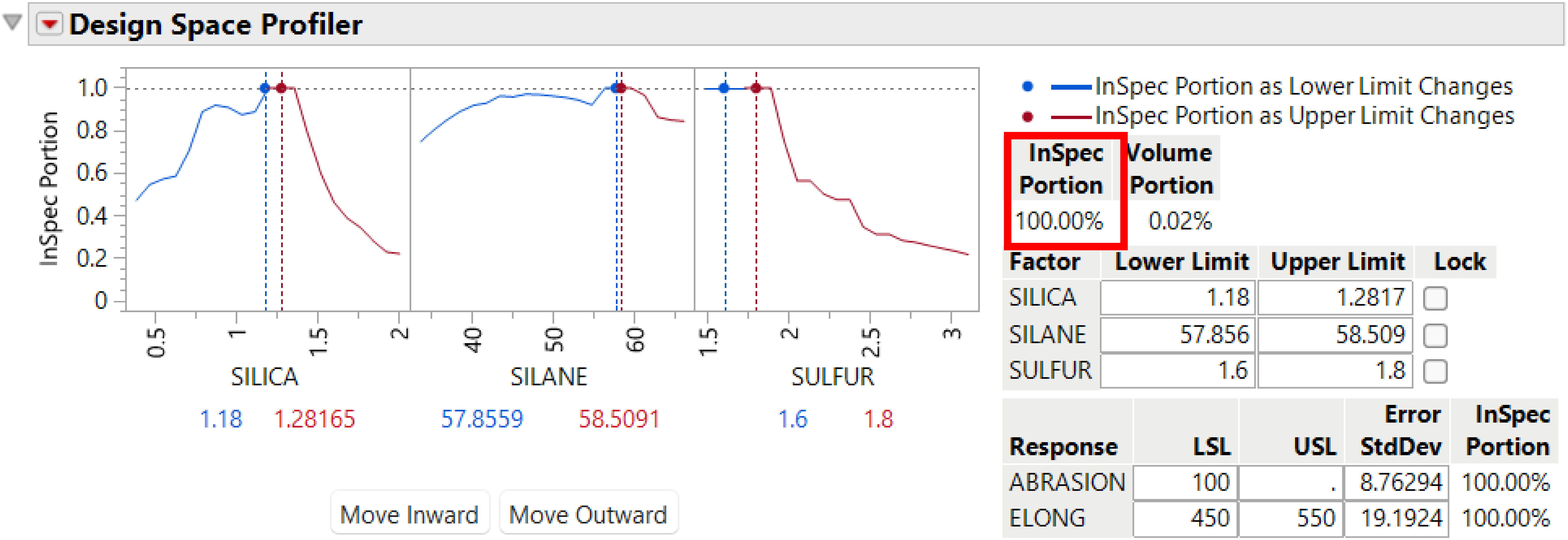


Bayesian Optimization



Launches the Design Space Profiler, which helps map specification limits on the Y variables to specification limits on the X variables.

Bayesian Optimization

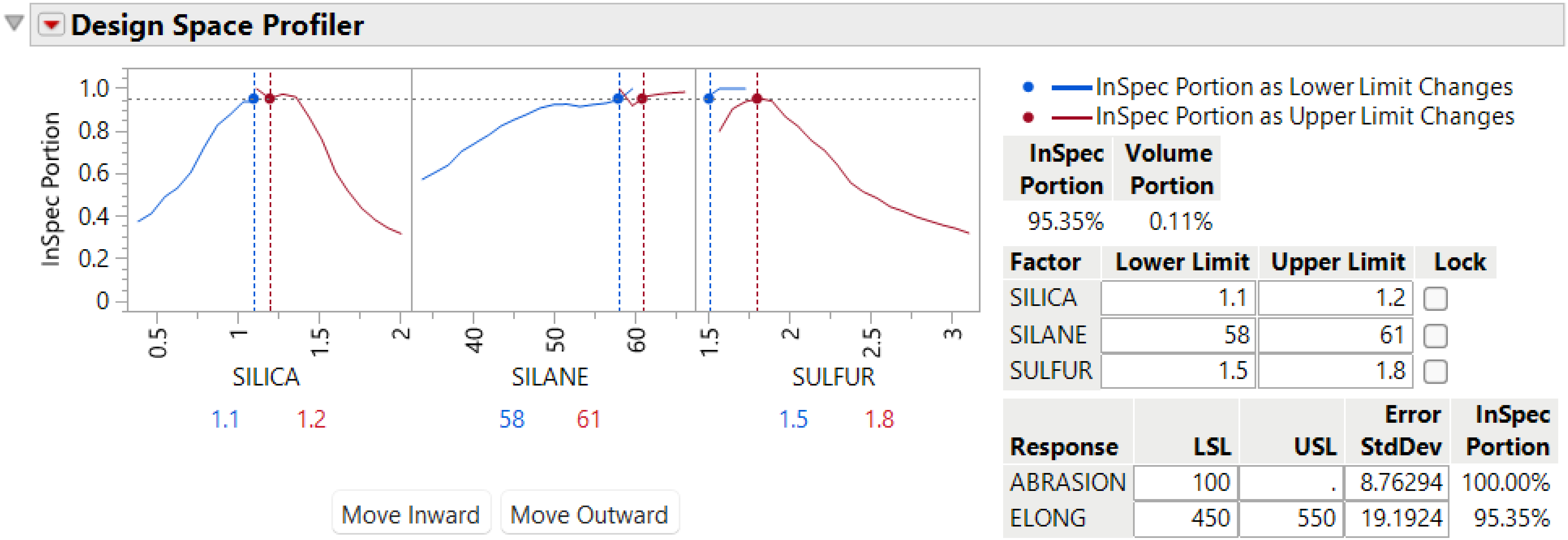


InSpec Portion	Volume Portion
100.00%	0.02%

Factor	Lower Limit	Upper Limit	Lock
SILICA	1.18	1.2817	☐
SILANE	57.856	58.509	☐
SULFUR	1.6	1.8	☐

Response	LSL	USL	Error StdDev	InSpec Portion
ABRASION	100	.	8.76294	100.00%
ELONG	450	550	19.1924	100.00%

Bayesian Optimization



Design Space Profiler

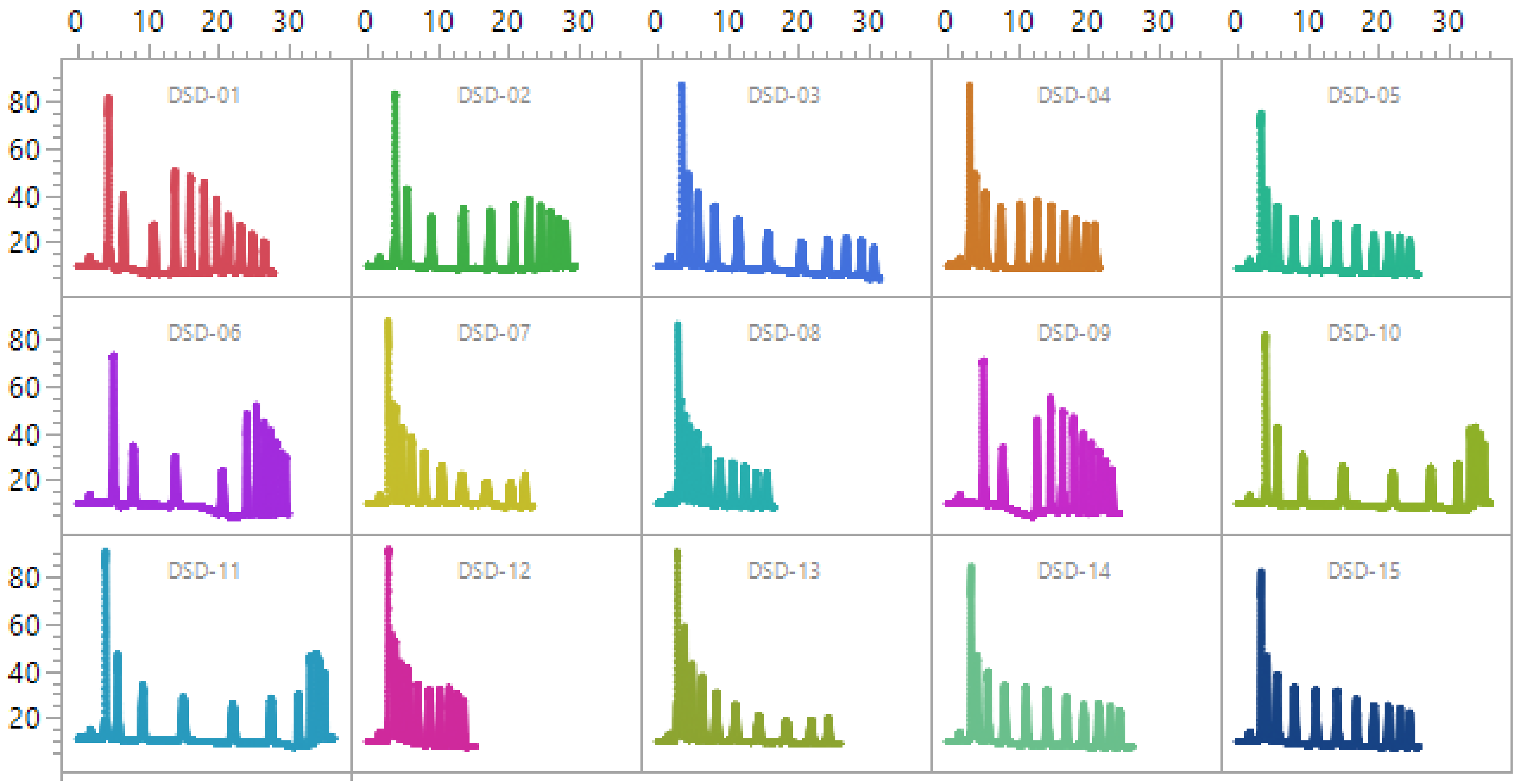
● InSpec Portion as Lower Limit Changes
● InSpec Portion as Upper Limit Changes

InSpec Portion	Volume Portion
95.35%	0.11%

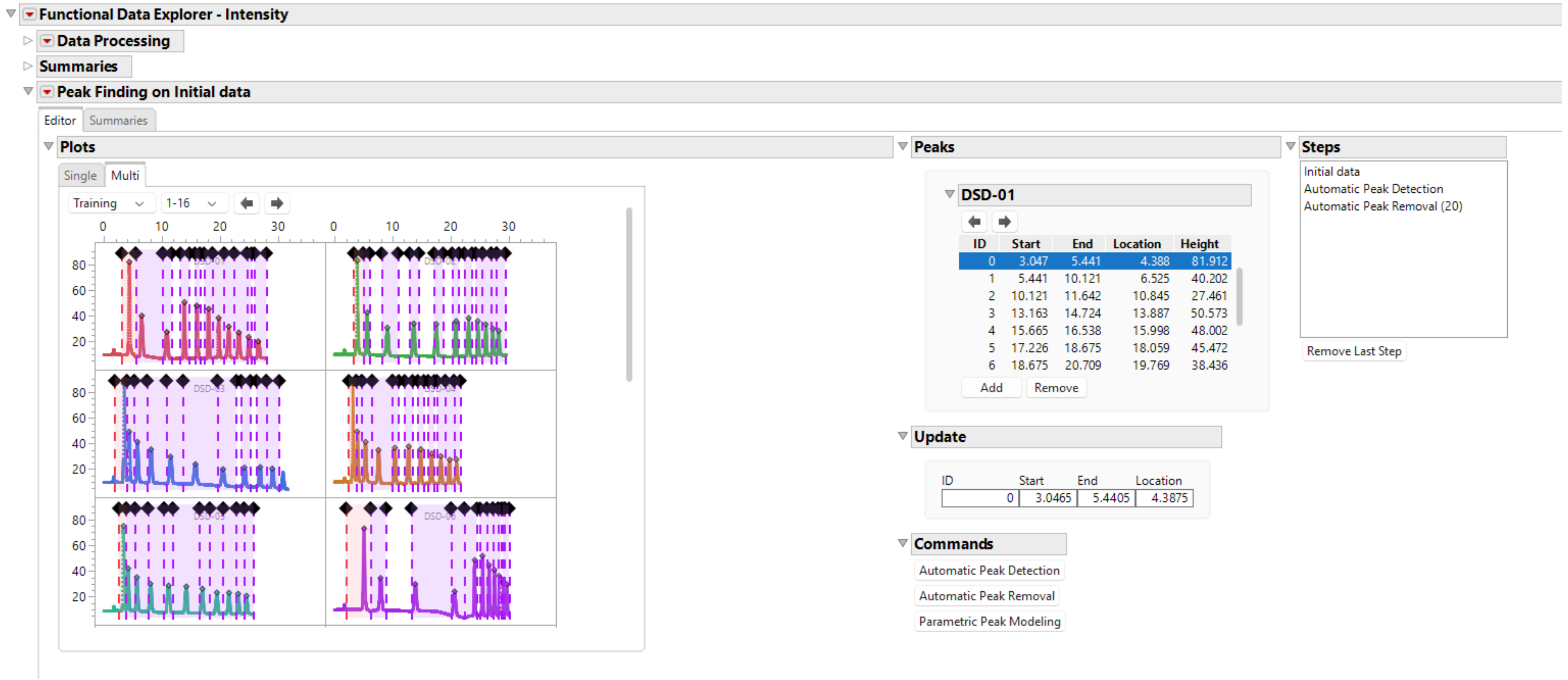
Factor	Lower Limit	Upper Limit	Lock
SILICA	1.1	1.2	☐
SILANE	58	61	☐
SULFUR	1.5	1.8	☐

Response	LSL	USL	Error StdDev	InSpec Portion
ABRASION	100	.	8.76294	100.00%
ELONG	450	550	19.1924	95.35%

Bayesian Optimization



Bayesian Optimization



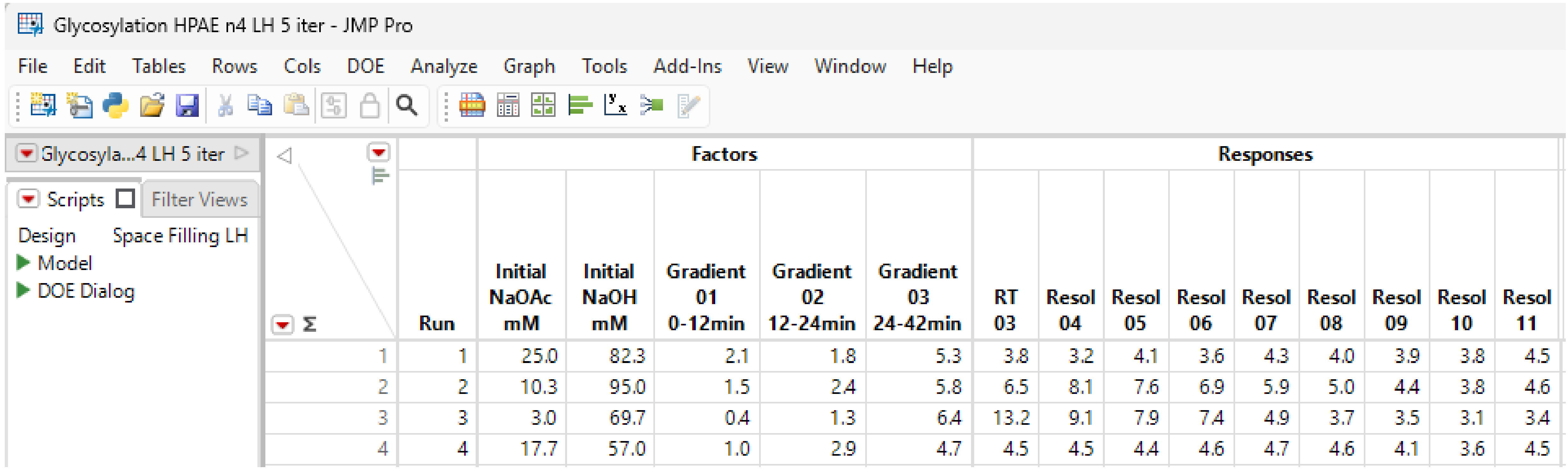
DSD-01

ID	Start	End	Location	Height
0	3.047	5.441	4.388	81.912
1	5.441	10.121	6.525	40.202
2	10.121	11.642	10.845	27.461
3	13.163	14.724	13.887	50.573
4	15.665	16.538	15.998	48.002
5	17.226	18.675	18.059	45.472
6	18.675	20.709	19.769	38.436

Steps
- Initial data
- Automatic Peak Detection
- Automatic Peak Removal (20)

Update

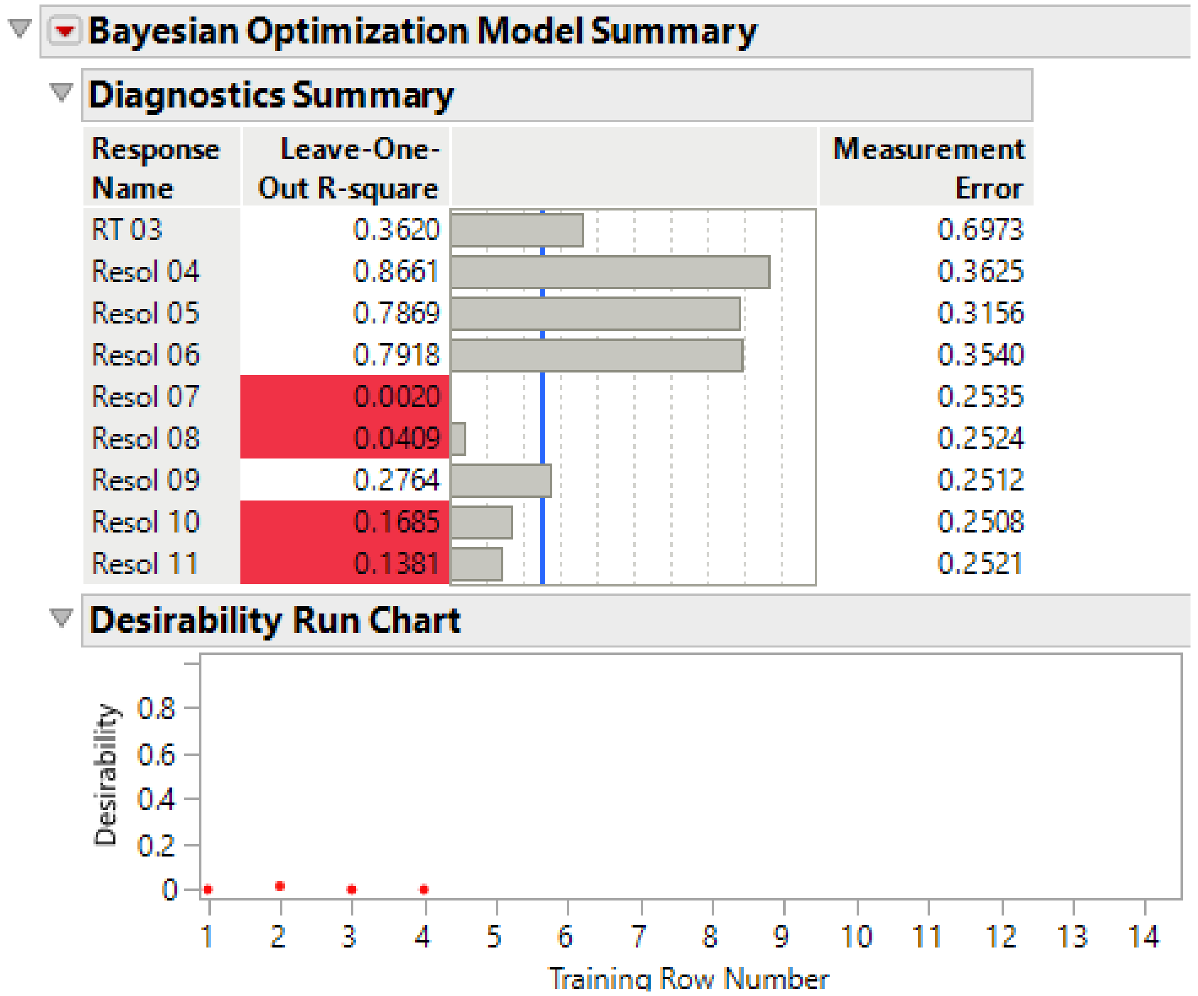
ID	Start	End	Location
0	3.0465	5.4405	4.3875



Design Space Filling LH

		Factors					Responses								
	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5

Bayesian Optimization

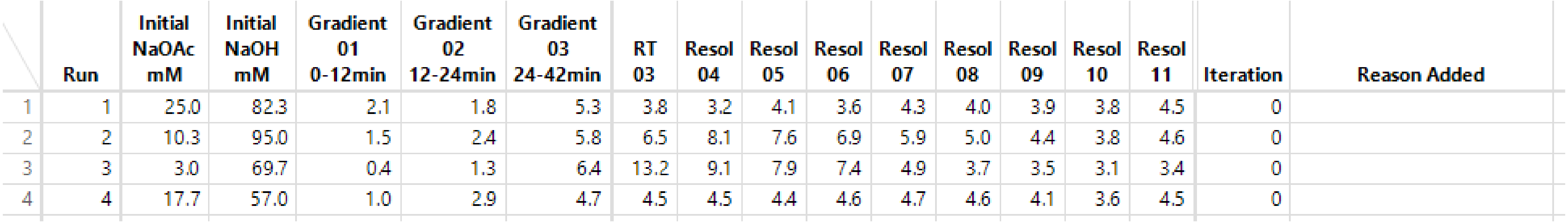


Bayesian Optimization Model Summary

Diagnostics Summary

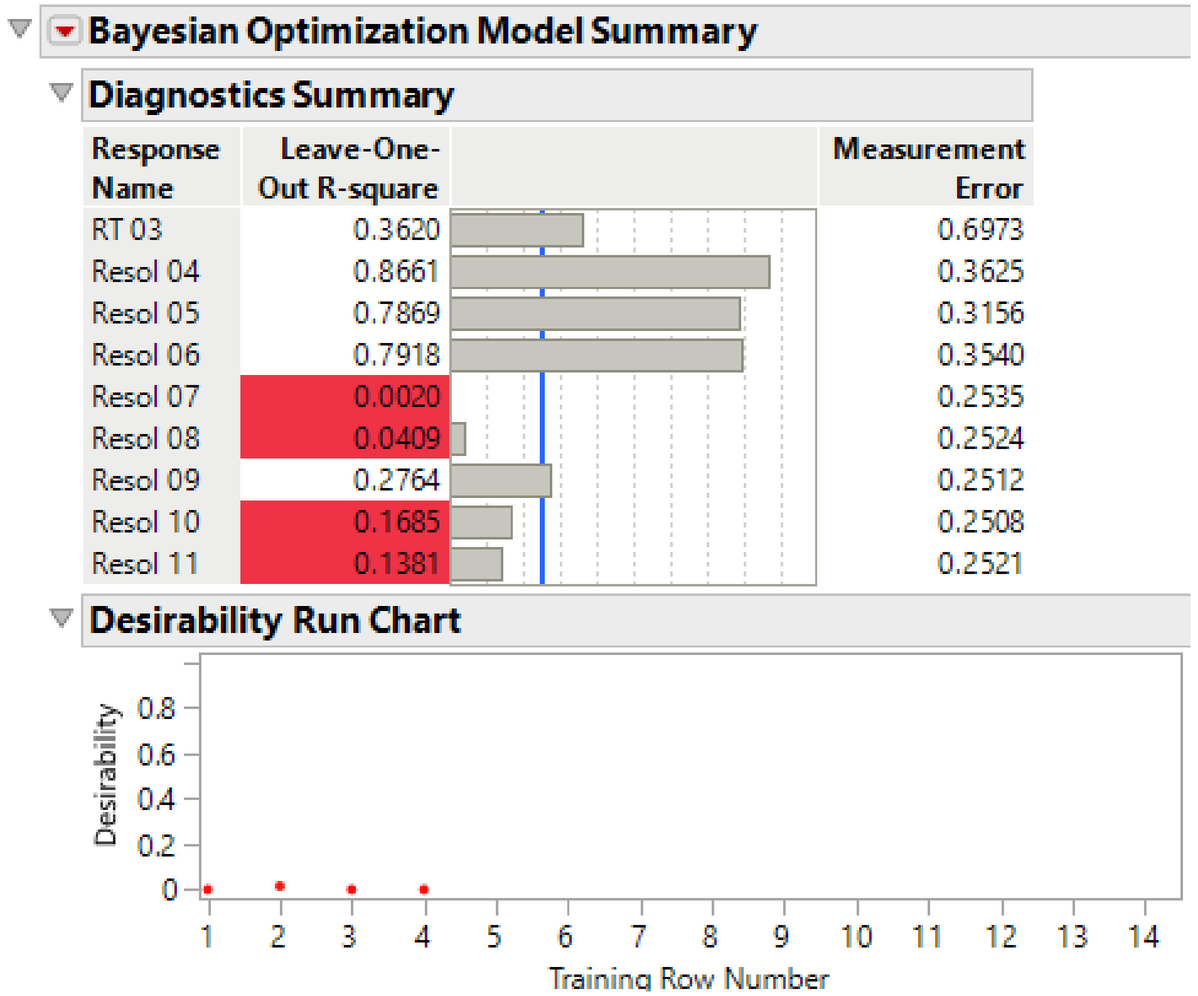
Response Name	Leave-One-Out R-square	Measurement Error
RT 03	0.3620	0.6973
Resol 04	0.8661	0.3625
Resol 05	0.7869	0.3156
Resol 06	0.7918	0.3540
Resol 07	0.0020	0.2535
Resol 08	0.0409	0.2524
Resol 09	0.2764	0.2512
Resol 10	0.1685	0.2508
Resol 11	0.1381	0.2521

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	

Bayesian Optimization

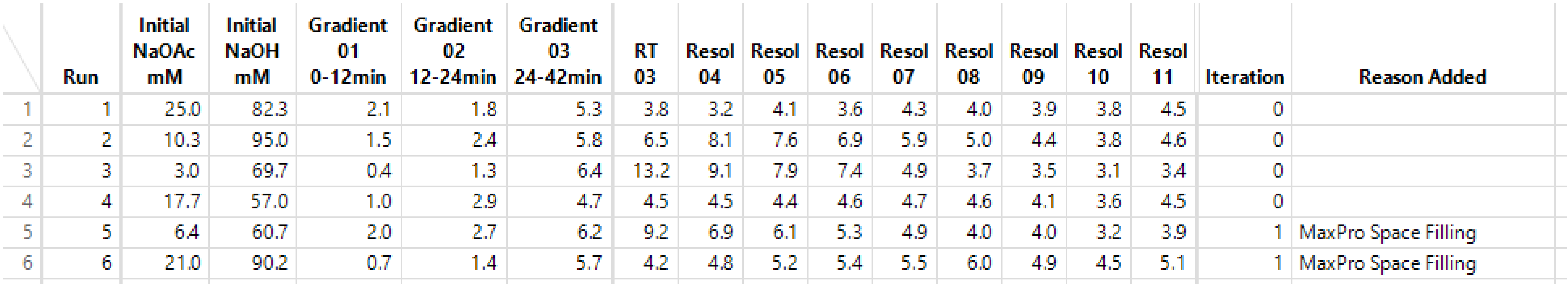


Bayesian Optimization Model Summary

Diagnostics Summary

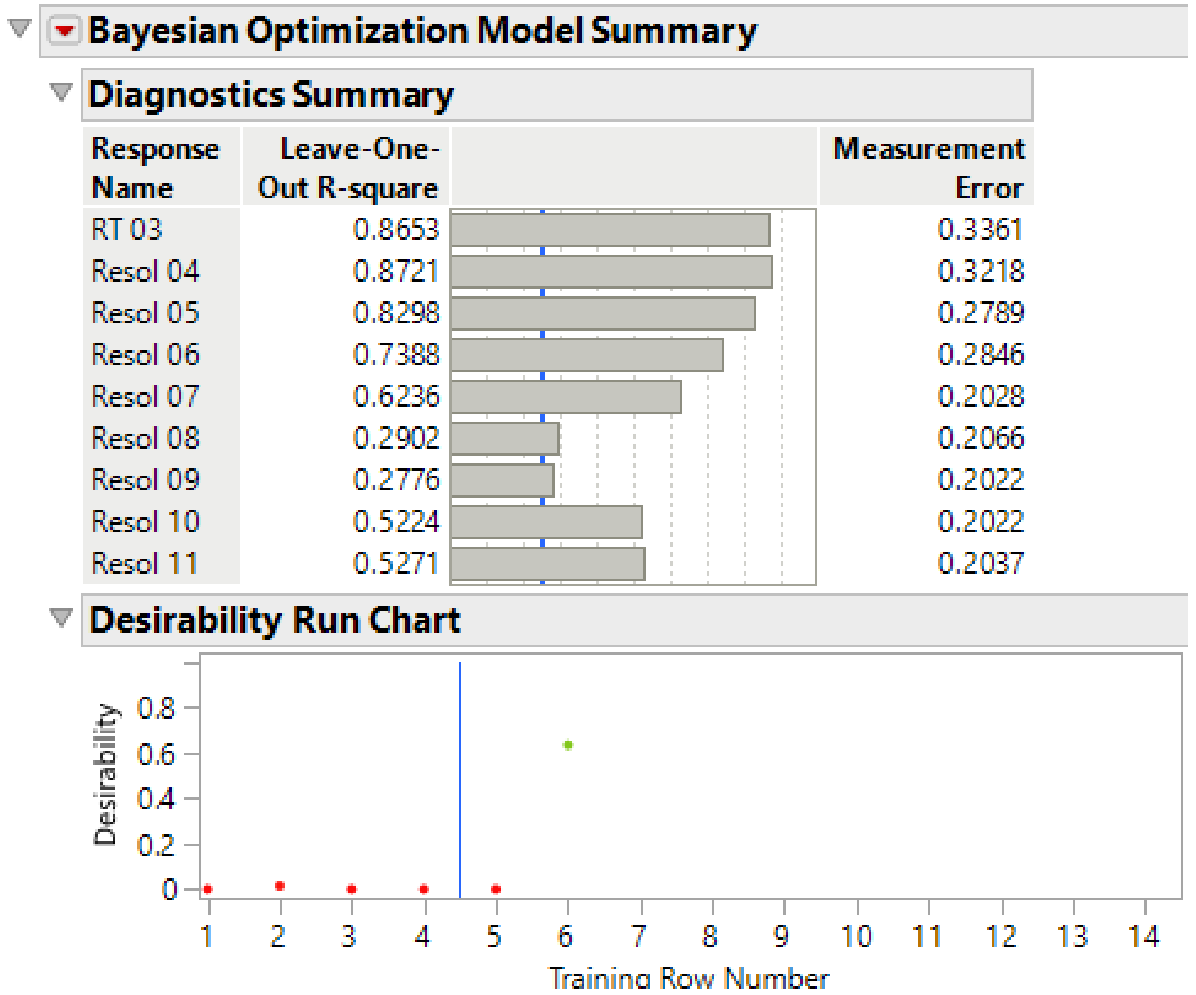
Response Name	Leave-One-Out R-square	Measurement Error
RT 03	0.3620	0.6973
Resol 04	0.8661	0.3625
Resol 05	0.7869	0.3156
Resol 06	0.7918	0.3540
Resol 07	0.0020	0.2535
Resol 08	0.0409	0.2524
Resol 09	0.2764	0.2512
Resol 10	0.1685	0.2508
Resol 11	0.1381	0.2521

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	
5	5	6.4	60.7	2.0	2.7	6.2	9.2	6.9	6.1	5.3	4.9	4.0	4.0	3.2	3.9	1	MaxPro Space Filling
6	6	21.0	90.2	0.7	1.4	5.7	4.2	4.8	5.2	5.4	5.5	6.0	4.9	4.5	5.1	1	MaxPro Space Filling

Bayesian Optimization

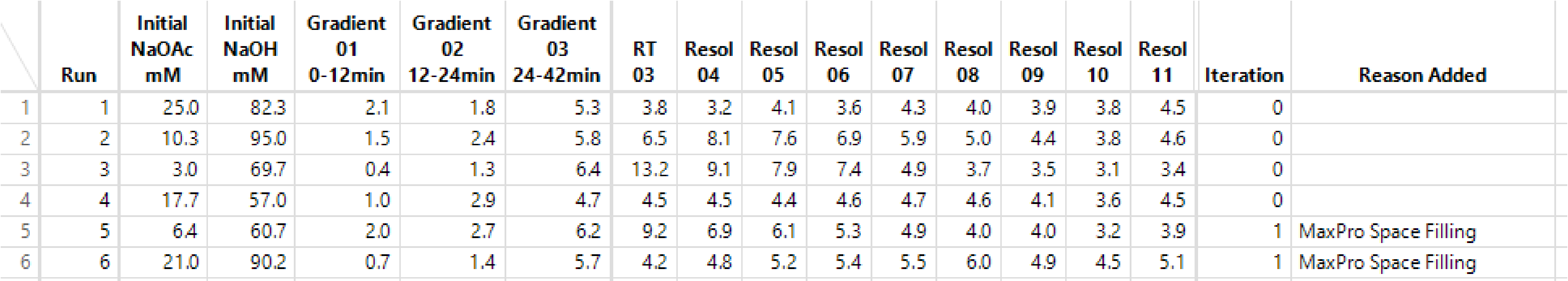


Bayesian Optimization Model Summary

Diagnostics Summary

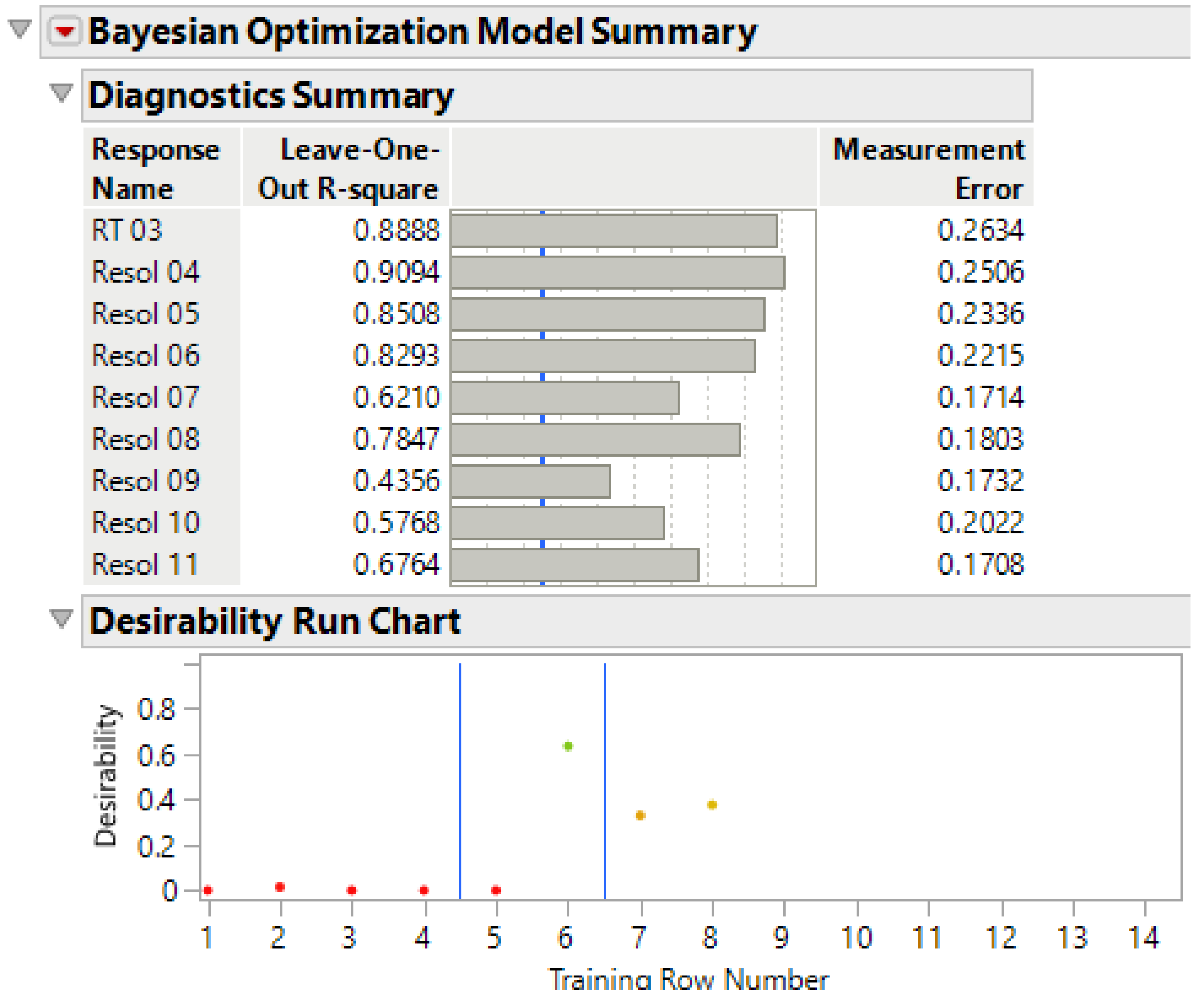
Response Name	Leave-One-Out R-square	Measurement Error
RT 03	0.8653	0.3361
Resol 04	0.8721	0.3218
Resol 05	0.8298	0.2789
Resol 06	0.7388	0.2846
Resol 07	0.6236	0.2028
Resol 08	0.2902	0.2066
Resol 09	0.2776	0.2022
Resol 10	0.5224	0.2022
Resol 11	0.5271	0.2037

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	
5	5	6.4	60.7	2.0	2.7	6.2	9.2	6.9	6.1	5.3	4.9	4.0	4.0	3.2	3.9	1	MaxPro Space Filling
6	6	21.0	90.2	0.7	1.4	5.7	4.2	4.8	5.2	5.4	5.5	6.0	4.9	4.5	5.1	1	MaxPro Space Filling

Bayesian Optimization

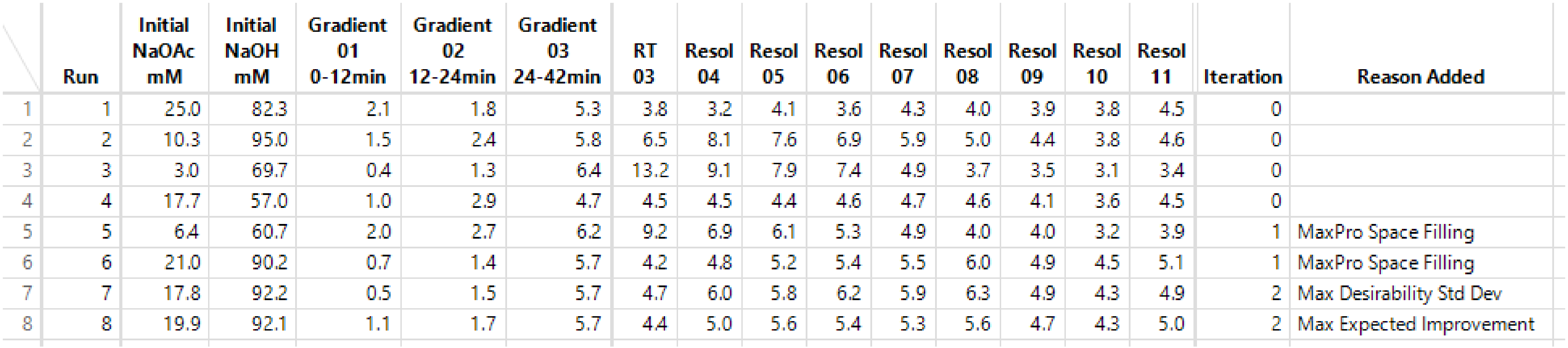


Bayesian Optimization Model Summary

Diagnostics Summary

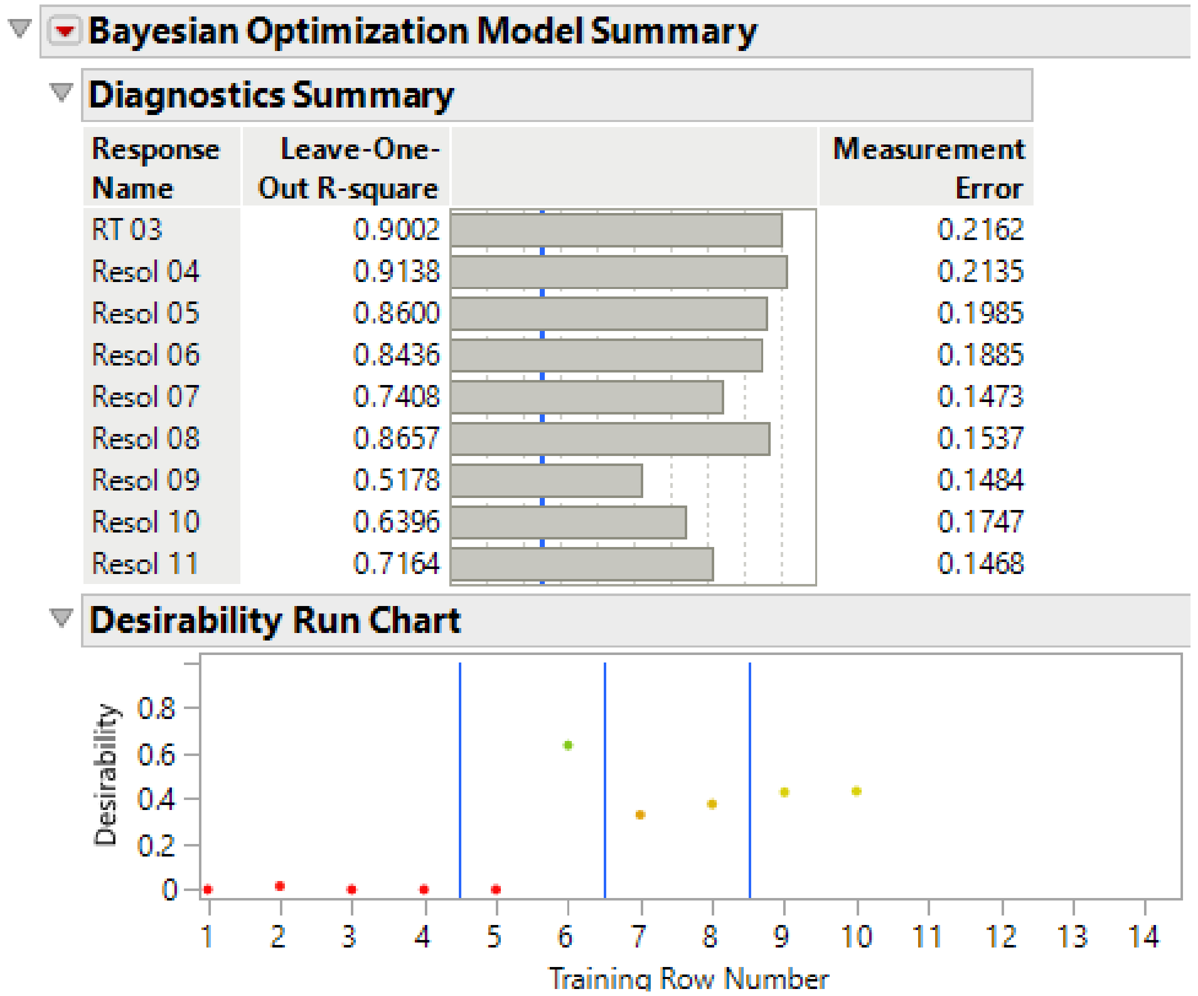
Response Name	Leave-One-Out R-square	Measurement Error
RT 03	0.8888	0.2634
Resol 04	0.9094	0.2506
Resol 05	0.8508	0.2336
Resol 06	0.8293	0.2215
Resol 07	0.6210	0.1714
Resol 08	0.7847	0.1803
Resol 09	0.4356	0.1732
Resol 10	0.5768	0.2022
Resol 11	0.6764	0.1708

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	
5	5	6.4	60.7	2.0	2.7	6.2	9.2	6.9	6.1	5.3	4.9	4.0	4.0	3.2	3.9	1	MaxPro Space Filling
6	6	21.0	90.2	0.7	1.4	5.7	4.2	4.8	5.2	5.4	5.5	6.0	4.9	4.5	5.1	1	MaxPro Space Filling
7	7	17.8	92.2	0.5	1.5	5.7	4.7	6.0	5.8	6.2	5.9	6.3	4.9	4.3	4.9	2	Max Desirability Std Dev
8	8	19.9	92.1	1.1	1.7	5.7	4.4	5.0	5.6	5.4	5.3	5.6	4.7	4.3	5.0	2	Max Expected Improvement

Bayesian Optimization

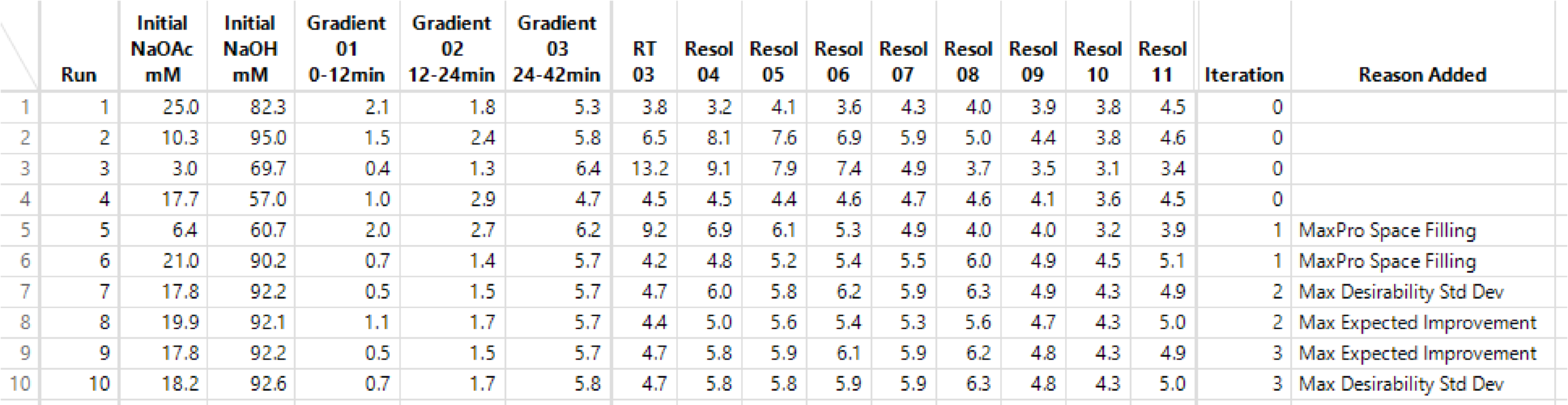


Bayesian Optimization Model Summary

Diagnostics Summary

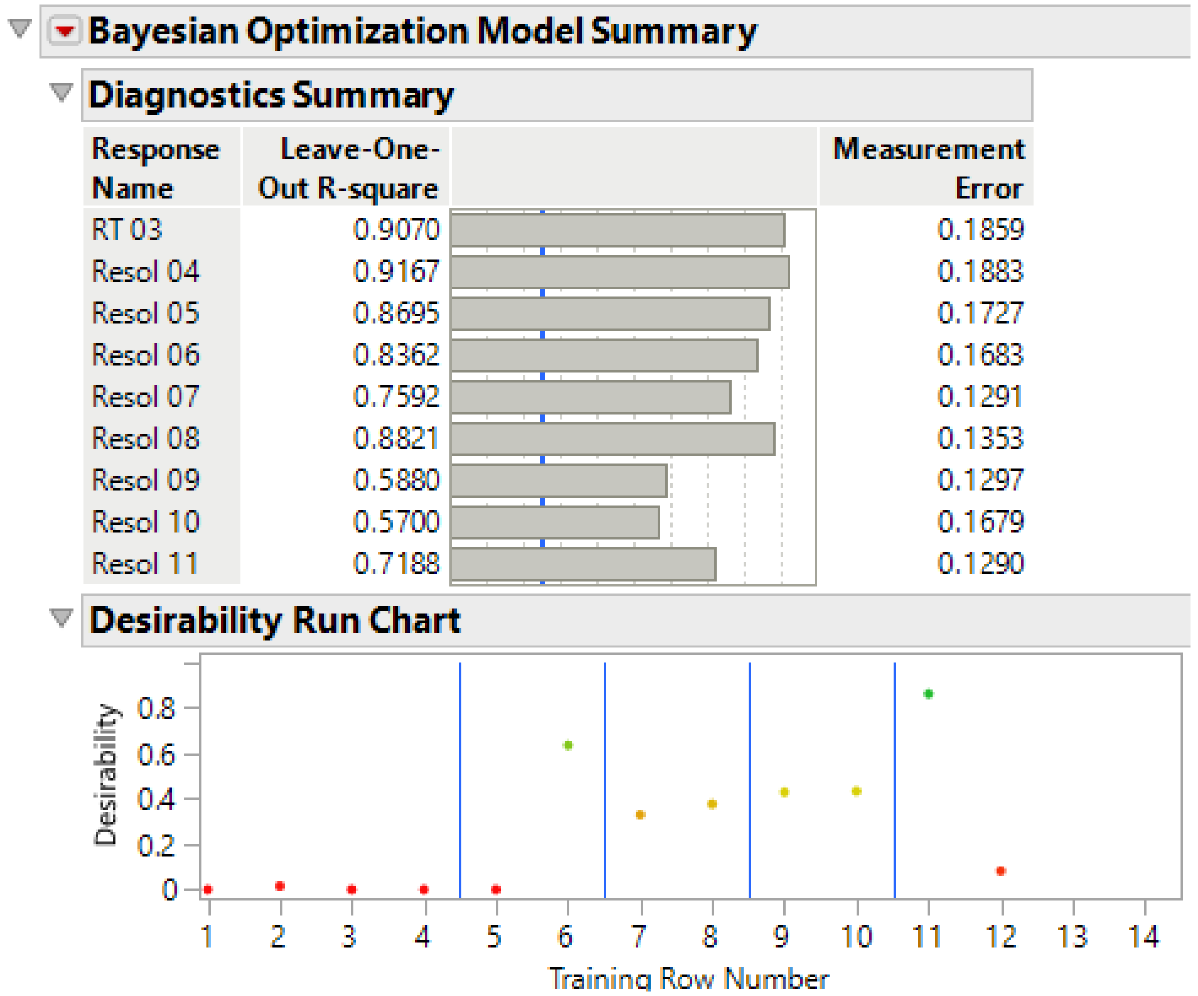
Response Name	Leave-One-Out R-square	Measurement Error
RT 03	0.9002	0.2162
Resol 04	0.9138	0.2135
Resol 05	0.8600	0.1985
Resol 06	0.8436	0.1885
Resol 07	0.7408	0.1473
Resol 08	0.8657	0.1537
Resol 09	0.5178	0.1484
Resol 10	0.6396	0.1747
Resol 11	0.7164	0.1468

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	
5	5	6.4	60.7	2.0	2.7	6.2	9.2	6.9	6.1	5.3	4.9	4.0	4.0	3.2	3.9	1	MaxPro Space Filling
6	6	21.0	90.2	0.7	1.4	5.7	4.2	4.8	5.2	5.4	5.5	6.0	4.9	4.5	5.1	1	MaxPro Space Filling
7	7	17.8	92.2	0.5	1.5	5.7	4.7	6.0	5.8	6.2	5.9	6.3	4.9	4.3	4.9	2	Max Desirability Std Dev
8	8	19.9	92.1	1.1	1.7	5.7	4.4	5.0	5.6	5.4	5.3	5.6	4.7	4.3	5.0	2	Max Expected Improvement
9	9	17.8	92.2	0.5	1.5	5.7	4.7	5.8	5.9	6.1	5.9	6.2	4.8	4.3	4.9	3	Max Expected Improvement
10	10	18.2	92.6	0.7	1.7	5.8	4.7	5.8	5.8	5.9	5.9	6.3	4.8	4.3	5.0	3	Max Desirability Std Dev

Bayesian Optimization

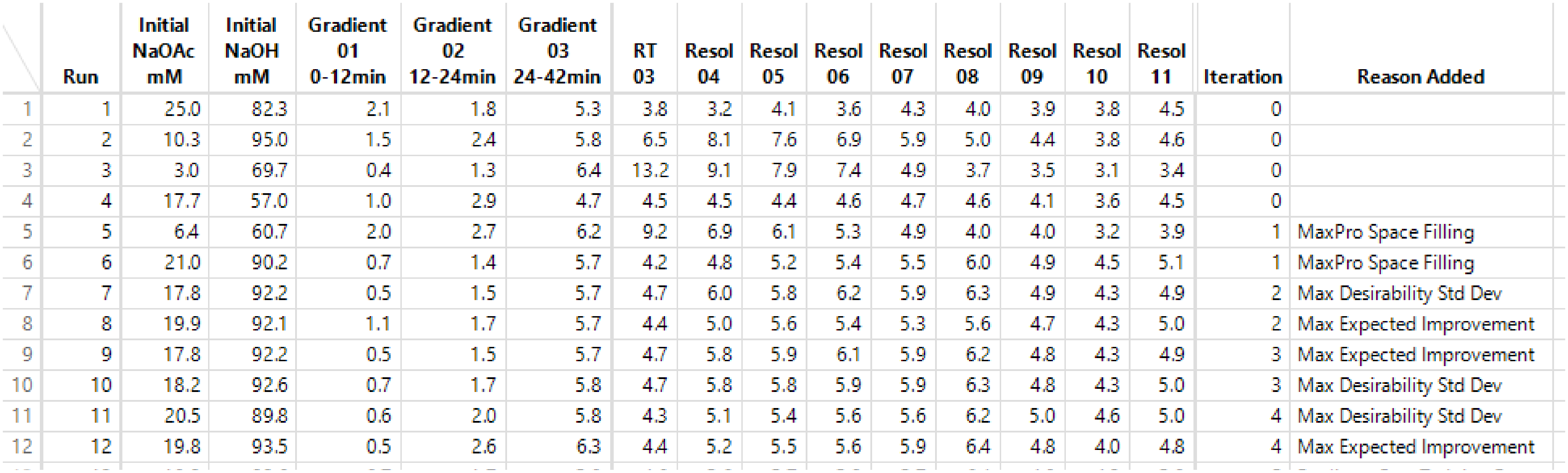


Bayesian Optimization Model Summary

Diagnostics Summary

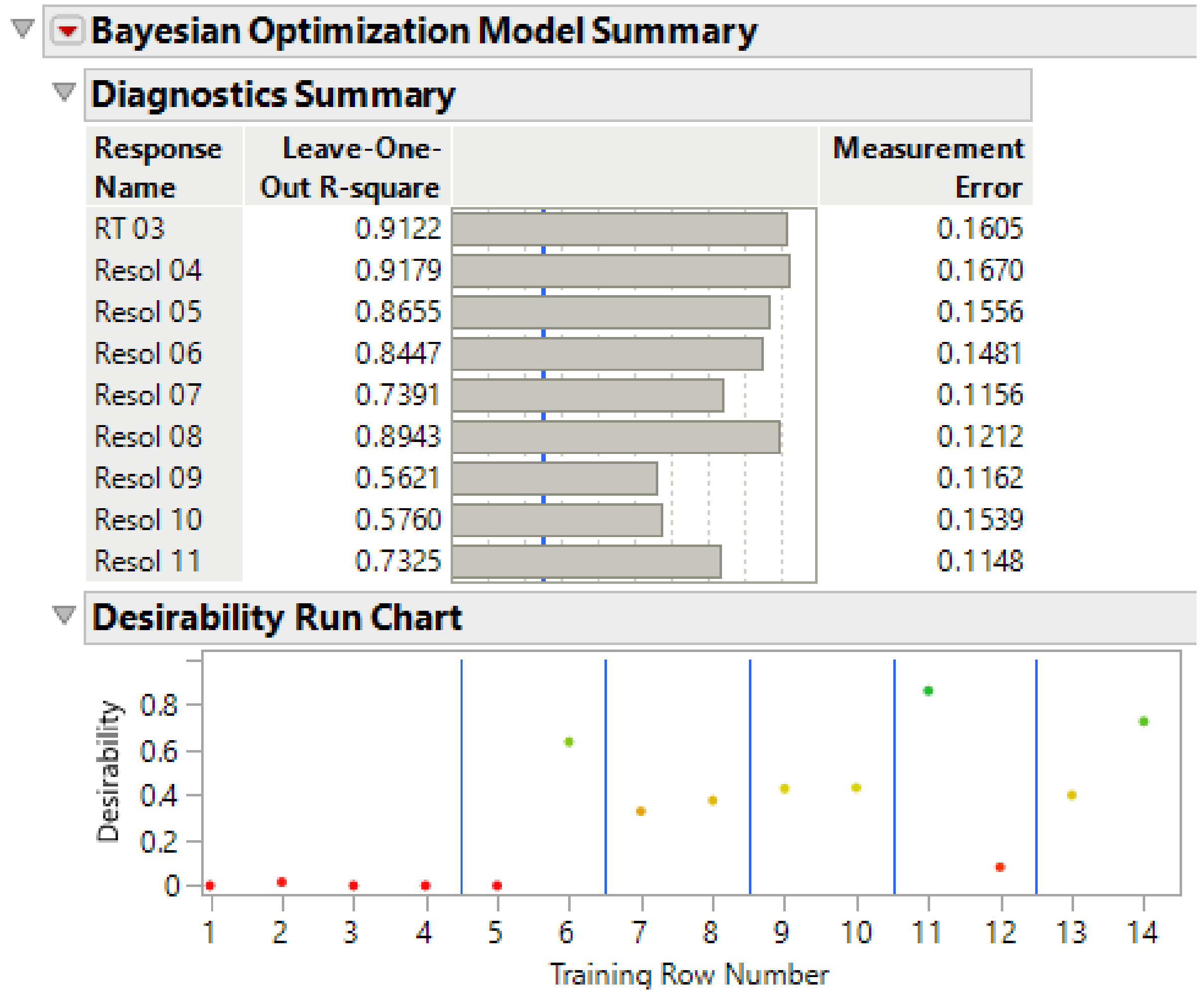
Response Name	Leave-One-Out R-square	Measurement Error
RT 03	0.9070	0.1859
Resol 04	0.9167	0.1883
Resol 05	0.8695	0.1727
Resol 06	0.8362	0.1683
Resol 07	0.7592	0.1291
Resol 08	0.8821	0.1353
Resol 09	0.5880	0.1297
Resol 10	0.5700	0.1679
Resol 11	0.7188	0.1290

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	
5	5	6.4	60.7	2.0	2.7	6.2	9.2	6.9	6.1	5.3	4.9	4.0	4.0	3.2	3.9	1	MaxPro Space Filling
6	6	21.0	90.2	0.7	1.4	5.7	4.2	4.8	5.2	5.4	5.5	6.0	4.9	4.5	5.1	1	MaxPro Space Filling
7	7	17.8	92.2	0.5	1.5	5.7	4.7	6.0	5.8	6.2	5.9	6.3	4.9	4.3	4.9	2	Max Desirability Std Dev
8	8	19.9	92.1	1.1	1.7	5.7	4.4	5.0	5.6	5.4	5.3	5.6	4.7	4.3	5.0	2	Max Expected Improvement
9	9	17.8	92.2	0.5	1.5	5.7	4.7	5.8	5.9	6.1	5.9	6.2	4.8	4.3	4.9	3	Max Expected Improvement
10	10	18.2	92.6	0.7	1.7	5.8	4.7	5.8	5.8	5.9	5.9	6.3	4.8	4.3	5.0	3	Max Desirability Std Dev
11	11	20.5	89.8	0.6	2.0	5.8	4.3	5.1	5.4	5.6	5.6	6.2	5.0	4.6	5.0	4	Max Desirability Std Dev
12	12	19.8	93.5	0.5	2.6	6.3	4.4	5.2	5.5	5.6	5.9	6.4	4.8	4.0	4.8	4	Max Expected Improvement

Bayesian Optimization

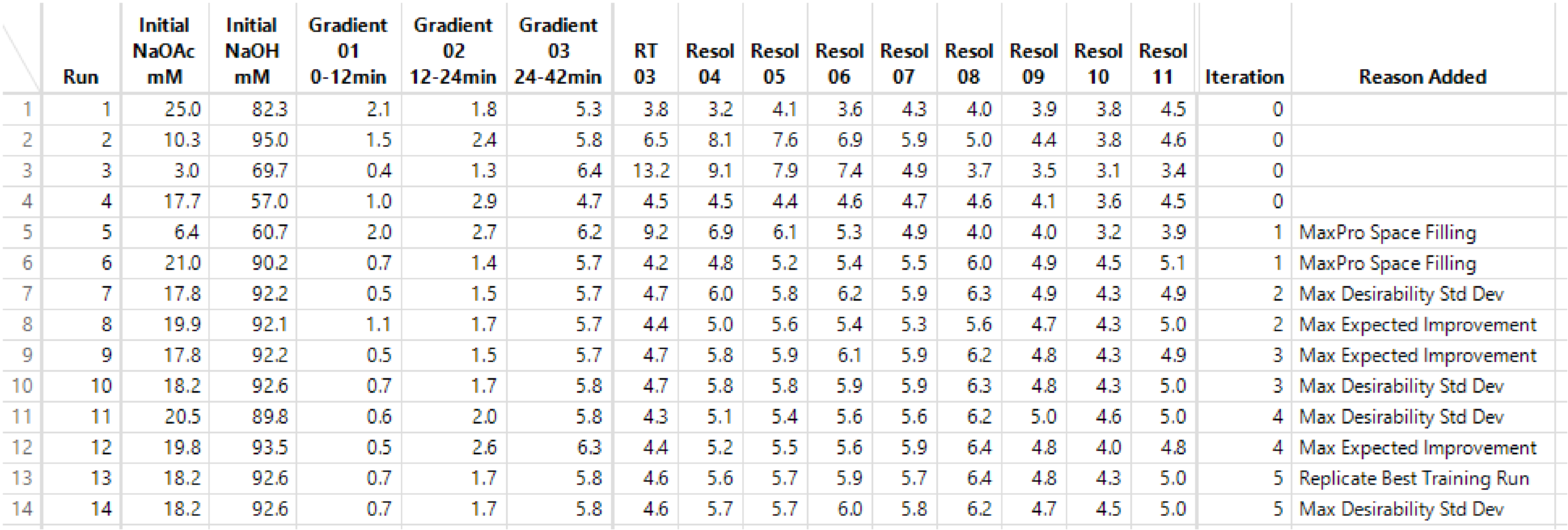


Bayesian Optimization Model Summary

Diagnostics Summary

Response Name	Leave-One-Out R-square		Measurement Error
RT 03	0.9122		0.1605
Resol 04	0.9179		0.1670
Resol 05	0.8655		0.1556
Resol 06	0.8447		0.1481
Resol 07	0.7391		0.1156
Resol 08	0.8943		0.1212
Resol 09	0.5621		0.1162
Resol 10	0.5760		0.1539
Resol 11	0.7325		0.1148

Desirability Run Chart



	Run	Initial NaOAc mM	Initial NaOH mM	Gradient 01 0-12min	Gradient 02 12-24min	Gradient 03 24-42min	RT 03	Resol 04	Resol 05	Resol 06	Resol 07	Resol 08	Resol 09	Resol 10	Resol 11	Iteration	Reason Added
1	1	25.0	82.3	2.1	1.8	5.3	3.8	3.2	4.1	3.6	4.3	4.0	3.9	3.8	4.5	0	
2	2	10.3	95.0	1.5	2.4	5.8	6.5	8.1	7.6	6.9	5.9	5.0	4.4	3.8	4.6	0	
3	3	3.0	69.7	0.4	1.3	6.4	13.2	9.1	7.9	7.4	4.9	3.7	3.5	3.1	3.4	0	
4	4	17.7	57.0	1.0	2.9	4.7	4.5	4.5	4.4	4.6	4.7	4.6	4.1	3.6	4.5	0	
5	5	6.4	60.7	2.0	2.7	6.2	9.2	6.9	6.1	5.3	4.9	4.0	4.0	3.2	3.9	1	MaxPro Space Filling
6	6	21.0	90.2	0.7	1.4	5.7	4.2	4.8	5.2	5.4	5.5	6.0	4.9	4.5	5.1	1	MaxPro Space Filling
7	7	17.8	92.2	0.5	1.5	5.7	4.7	6.0	5.8	6.2	5.9	6.3	4.9	4.3	4.9	2	Max Desirability Std Dev
8	8	19.9	92.1	1.1	1.7	5.7	4.4	5.0	5.6	5.4	5.3	5.6	4.7	4.3	5.0	2	Max Expected Improvement
9	9	17.8	92.2	0.5	1.5	5.7	4.7	5.8	5.9	6.1	5.9	6.2	4.8	4.3	4.9	3	Max Expected Improvement
10	10	18.2	92.6	0.7	1.7	5.8	4.7	5.8	5.8	5.9	5.9	6.3	4.8	4.3	5.0	3	Max Desirability Std Dev
11	11	20.5	89.8	0.6	2.0	5.8	4.3	5.1	5.4	5.6	5.6	6.2	5.0	4.6	5.0	4	Max Desirability Std Dev
12	12	19.8	93.5	0.5	2.6	6.3	4.4	5.2	5.5	5.6	5.9	6.4	4.8	4.0	4.8	4	Max Expected Improvement
13	13	18.2	92.6	0.7	1.7	5.8	4.6	5.6	5.7	5.9	5.7	6.4	4.8	4.3	5.0	5	Replicate Best Training Run
14	14	18.2	92.6	0.7	1.7	5.8	4.6	5.7	5.7	6.0	5.8	6.2	4.7	4.5	5.0	5	Max Desirability Std Dev

Bayesian Optimization