Functional Data Analysis (FDA) and Nonlinear Regression Models (NLR): an information quality perspective

March 22nd, 2022

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KPA Insights through analytics

jmp STATISTICAL DISCOVERY

Agenda

- A simple example – Ron
  - Intro to Functional Data Analysis (FDA)
  - Intro to Non-Linear Regression (NLR)
- An optimization example – Chris
  - Mixture experiments with profile responses
  - Designing tablets to match a reference profile

Dissolution Curves of 12 tablets. Test and Reference

	Time	Label R	Data R	Label T	Data T
1	5	T1R	72.7	T1	46.6
2	5	T2R	78.8	T2	10.5
3	5	T3R	32.3	T3	10
4	5	T4R	38.8	T4	42.9
5	5	T5R	18.9	T5	61
6	5	T6R	52.1	T6	36.3
7	5	T7R	14.3	T7	6.4
8	5	T8R	67.8	T8	4.4
9	5	T9R	7.5	T9	5.4
10	5	T10R	8.5	T10	3.6
11	5	T11R	26.5	T11	6.4
12	5	T12R	10.2	T12	35
13	10	T1R	89.1	T1	74
14	10	T2R	94.4	T2	38.1
15	10	T3R	60.5	T3	30.9
16	10	T4R	63.7	T4	88.1
17	10	T5R	31.3	T5	84.3
18	10	T6R	79.6	T6	71.9
19	10	T7R	44.3	T7	39.4

Test

Level	Count
5	12
10	12
15	12
20	12
30	12
45	12
Total	72

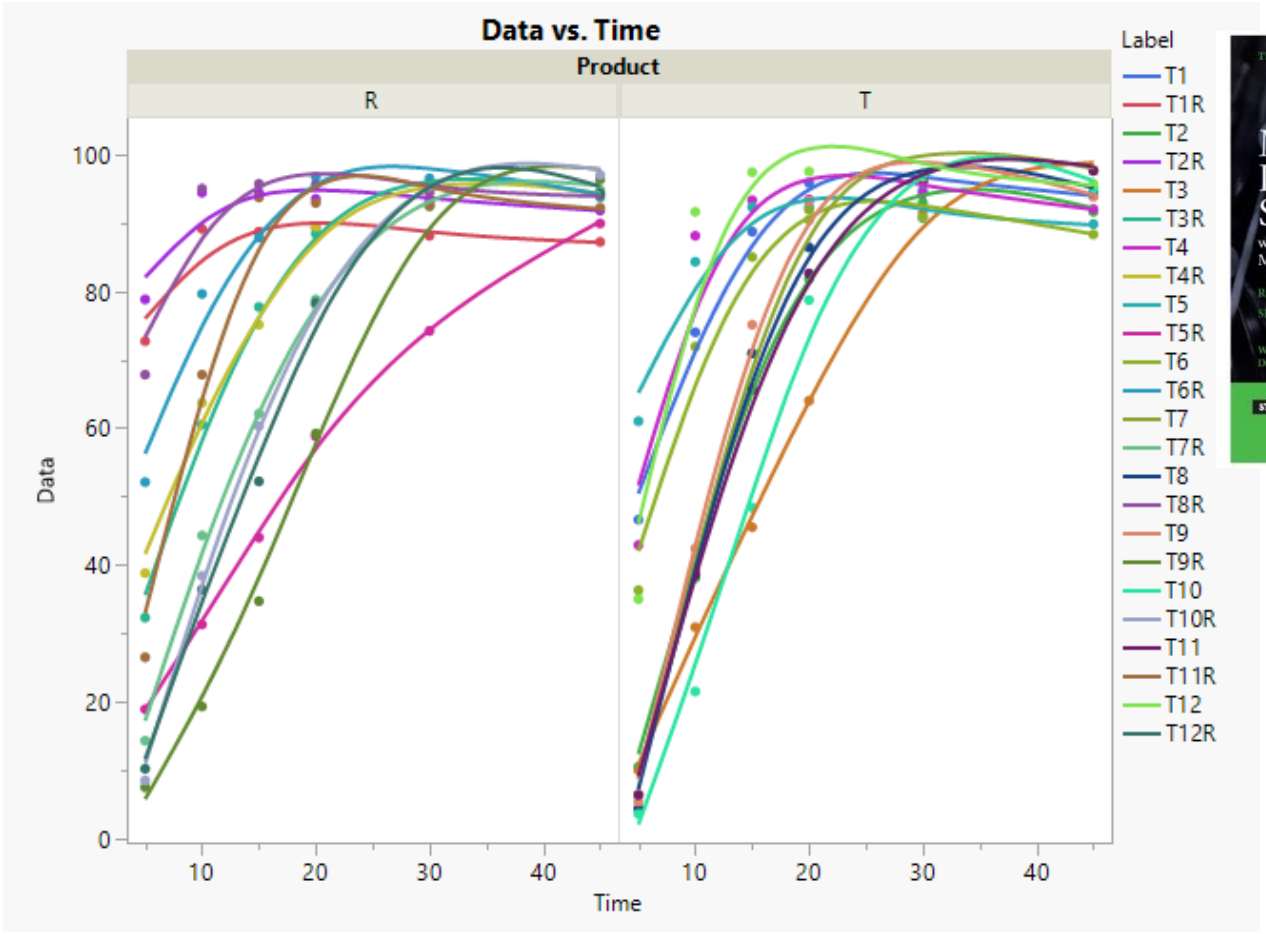
Reference

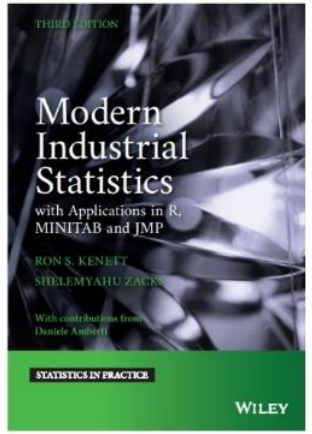
Level	Count
5	12
10	12
15	12
20	12
30	12
45	12
Total	72

FDA

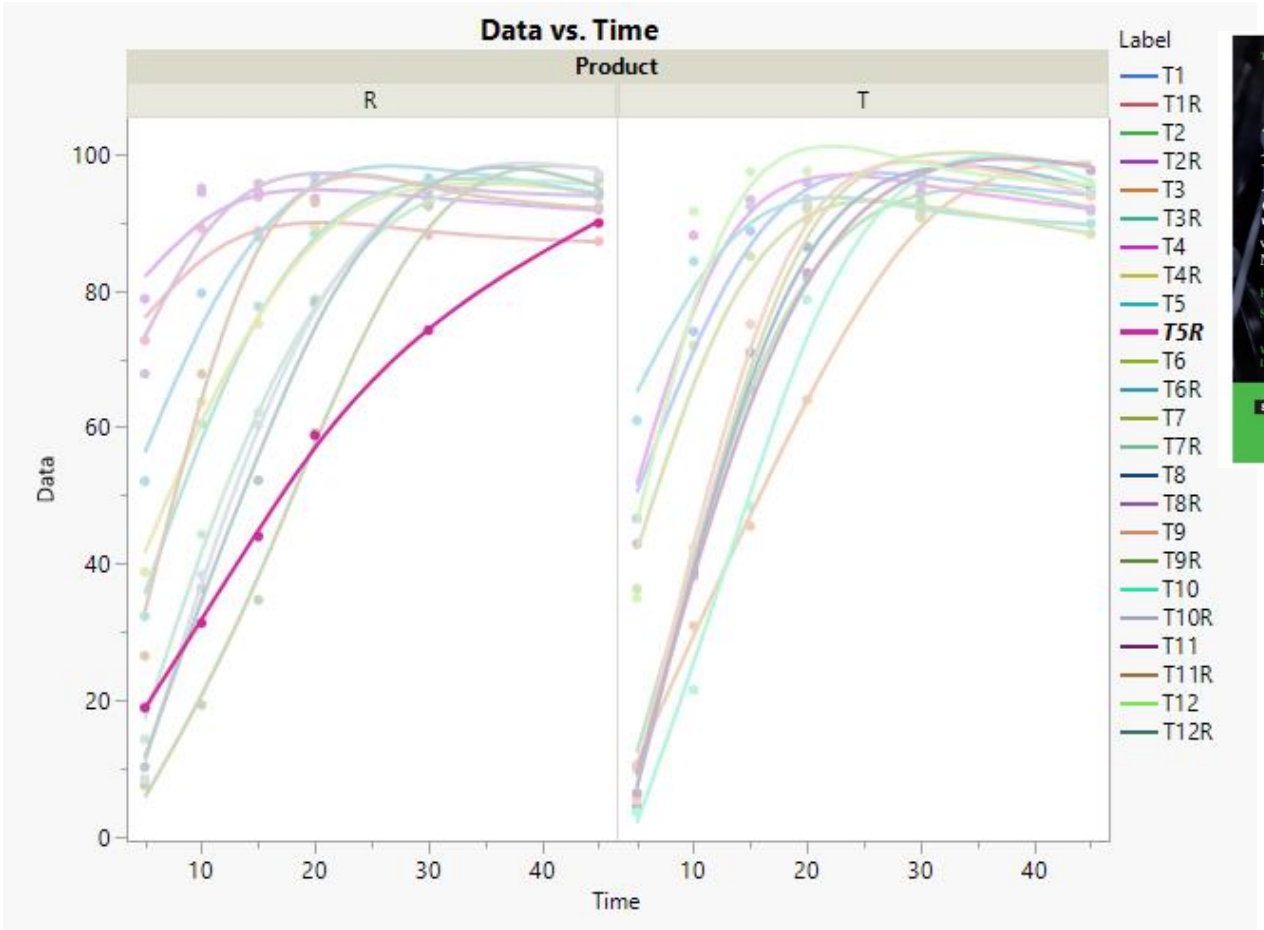
NLR

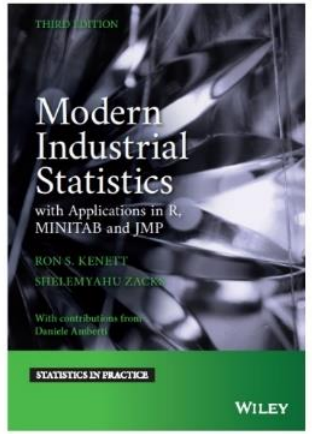
Dissolution Curves of 12 tablets. Test and Reference





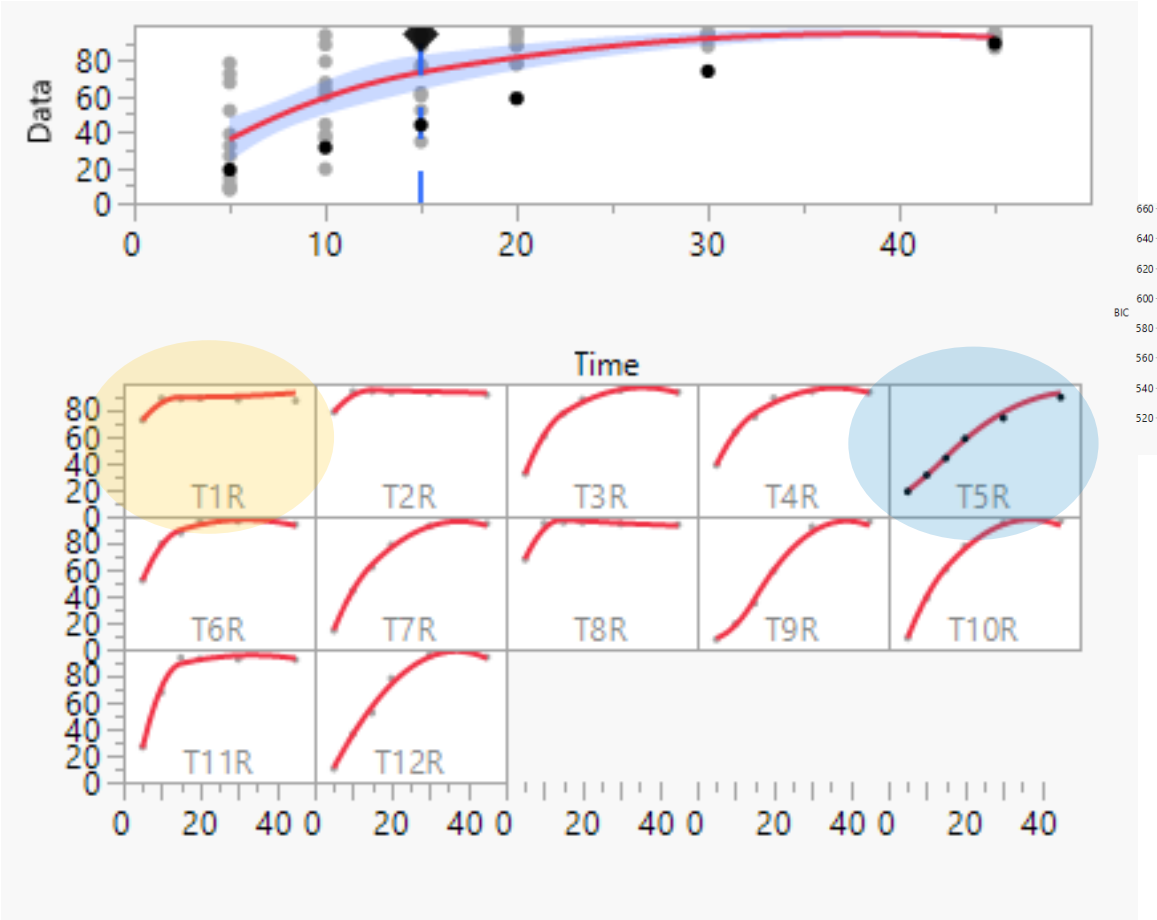
Dissolution Curves of 12 tablets. Test T5R Is different



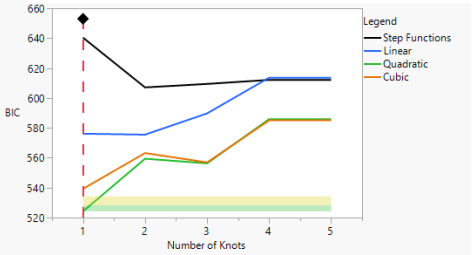


Dissolution Curves of 12 tablets.

Test T5R Is different



FDA

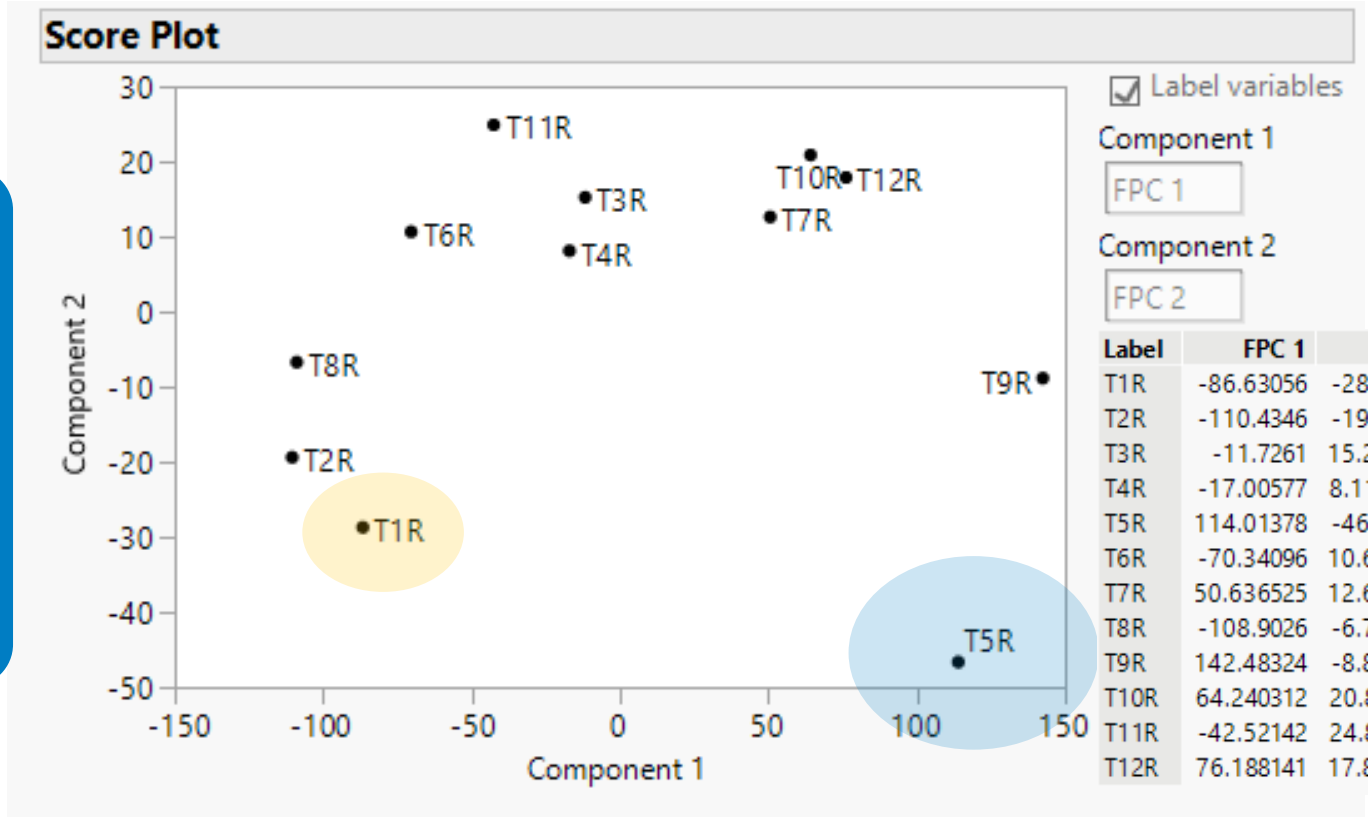


Quadratic B-spline with 1 knot

Dissolution Curves of 12 tablets.

Test T5R Is different

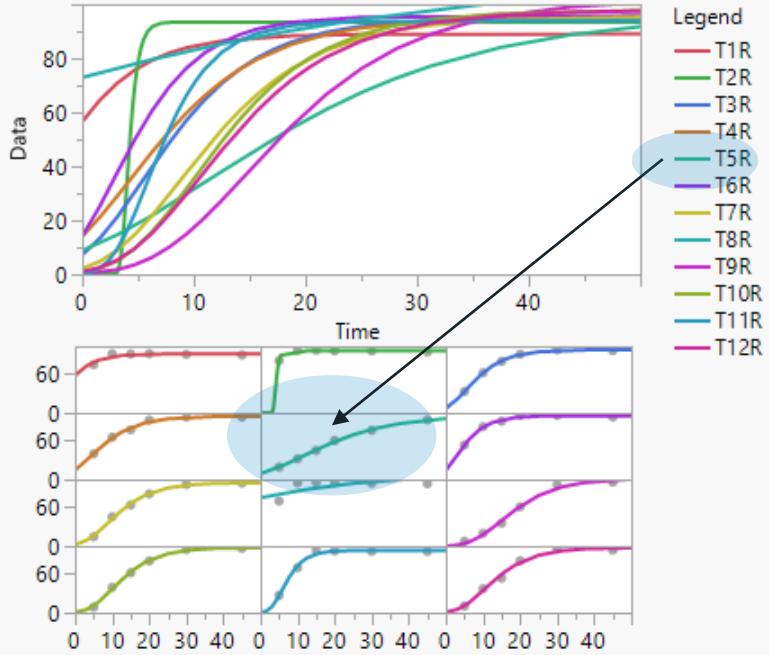
FDA



Label	FPC 1	FPC 2	FPC 3
T1R	-86.63056	-28.70704	0.996566
T2R	-110.4346	-19.38626	7.7488408
T3R	-11.7261	15.242747	0.0425637
T4R	-17.00577	8.1173121	3.7777815
T5R	114.01378	-46.64264	-12.92808
T6R	-70.34096	10.648925	3.9284304
T7R	50.636525	12.627046	-3.211241
T8R	-108.9026	-6.710816	0.0497409
T9R	142.48324	-8.840222	11.976841
T10R	64.240312	20.878974	-0.66174
T11R	-42.52142	24.890182	-18.14564
T12R	76.188141	17.881793	6.4259358

Gompertz 3P

Plot

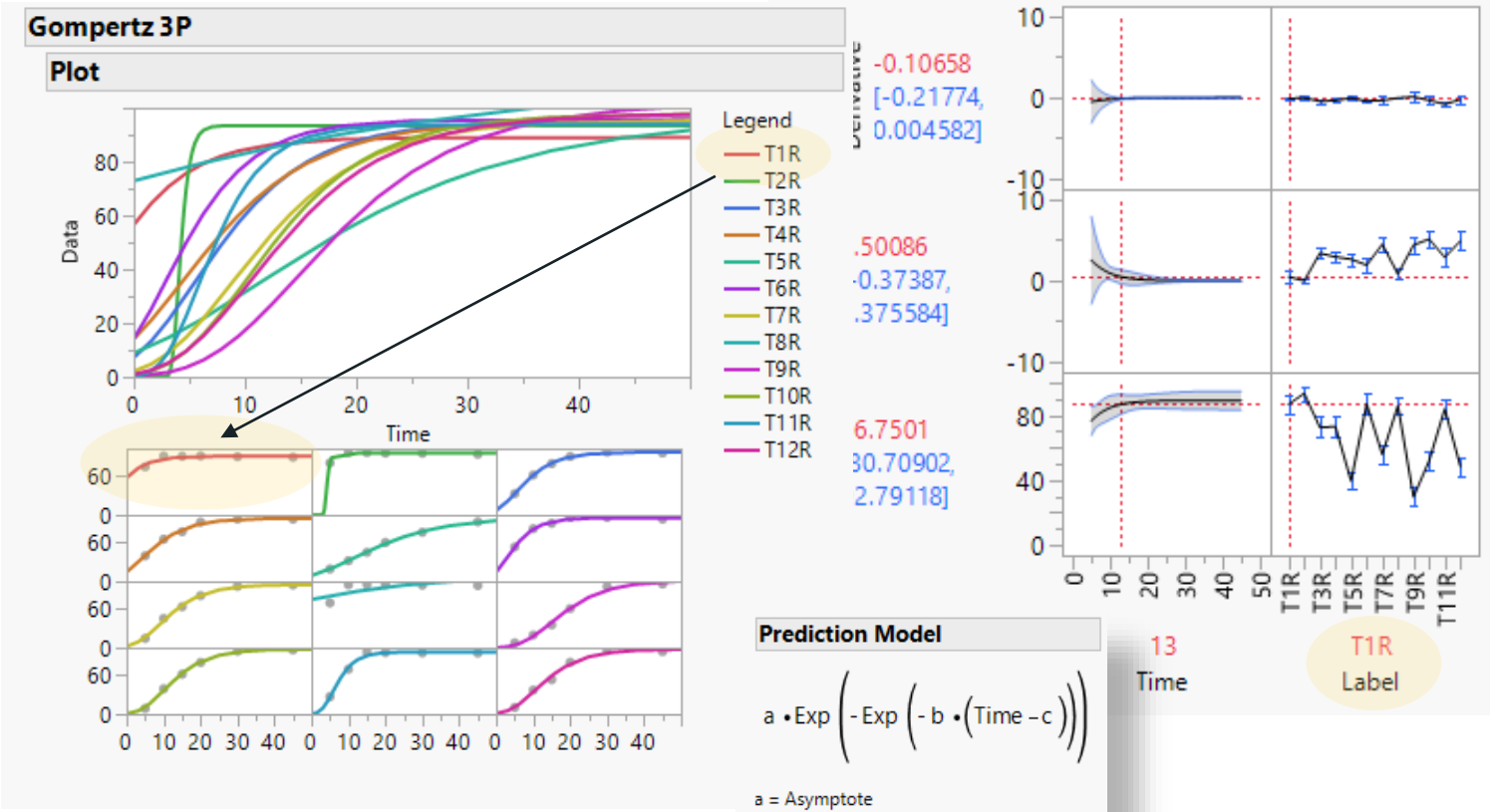


Prediction Model

$$a \bullet \mathrm{Exp}\left(-\mathrm{Exp}\left(-b \bullet (\mathrm{Time} - c)\right)\right)$$

a = Asymptote
b = Growth Rate
c = Inflection Point

NLR


Gompertz 3P
Plot
Data
Time
Legend
T1R
T2R
T3R
T4R
T5R
T6R
T7R
T8R
T9R
T10R
T11R
T12R
Prediction Profiler
-0.10658
[-0.21774,
0.004582]
.50086
-0.37387,
.375584]
6.7501
30.70902,
2.79118]
Prediction Model
a • Exp (- Exp (- b • (Time - c)))
a = Asymptote
b = Growth Rate
c = Inflection Point
13
Time
T1R
Label

NLR

	Label	Asymptote	Growth Rate	Inflection Point
T1R 1	T1R	89.072244404	0.2185624809	-3.625806907
2	T2R	93.480399791	1.76758908	4.0002987548
3	T3R	95.117117858	0.1732544061	5.4556204689
4	T4R	95.393703545	0.1508168903	4.2794474042
T5R 5	T5R	97.047132531	0.0750862269	11.579937352
6	T6R	95.886344295	0.2282099484	2.8239229453
7	T7R	95.608682945	0.1500953986	8.8540204547
8	T8R	113.26922091	0.0355126872	-23.11022674
9	T9R	102.16502758	0.1201635618	14.766362121
10	T10R	97.965019617	0.1562304451	10.087517474
11	T11R	94.032980681	0.3037771891	5.8648755174
12	T12R	97.966870258	0.1439240958	10.549169714

NLR

Prediction Model

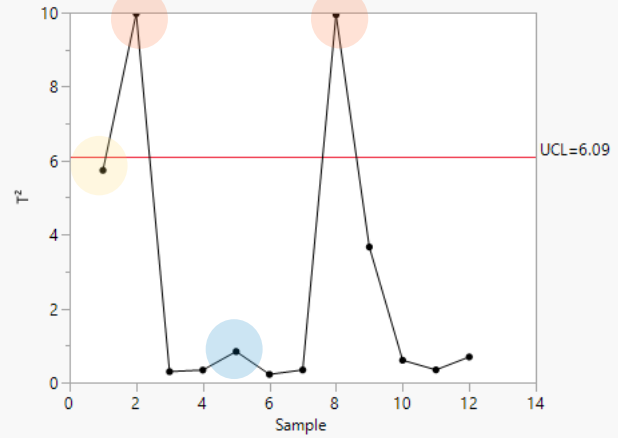
$$a \bullet \mathrm{Exp}\left(-\mathrm{Exp}\left(-b \bullet (\mathrm{Time} - c)\right)\right)$$

a = Asymptote
b = Growth Rate
c = Inflection Point

multivariate statistical distance (MSD)

Multivariate Control Chart

T Square with All Principal Components



Note: UCL is calculated based on Alpha=0.05

Principal Components: on Covariances

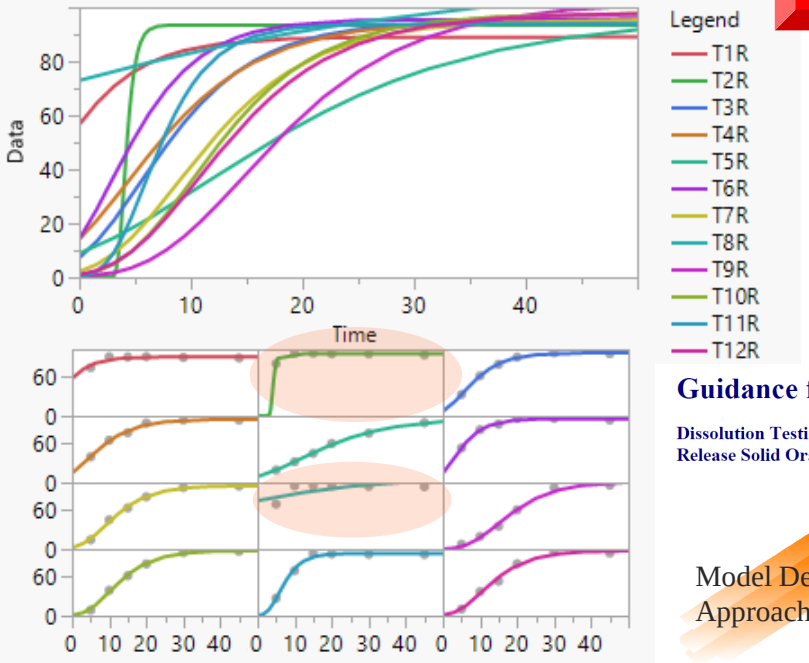
Eigenvalue	Percent	20 40 60 80	Cum Percent	ChiSquare	DF	Prob>ChiSq
109.6992	82.409		82.409	56.861	5.000	<.0001*
23.2208	17.444		99.853	37.506	2.000	<.0001*
0.1951	0.147		100.000	0.000	0.000	.

Eigenvectors			
Asymptote	-0.03538	0.19264	0.07053
Growth Rate	0.00038	-0.00663	2.26272
Inflection Point	0.08868	0.07689	0.01853

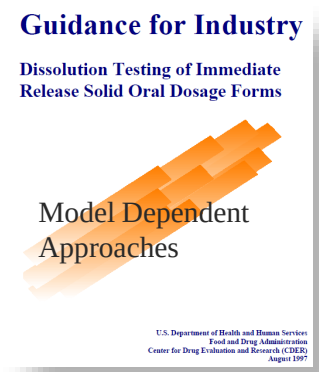
Note: Eigenvectors were divided by square root of eigenvalues.

Gompertz 3P

Plot

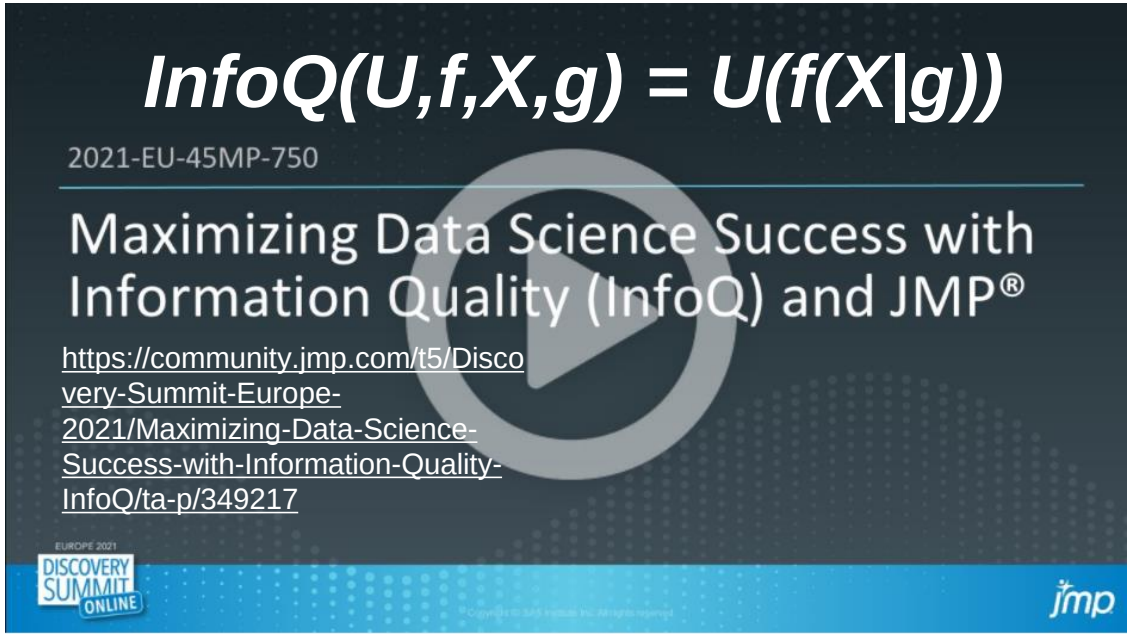


NLR

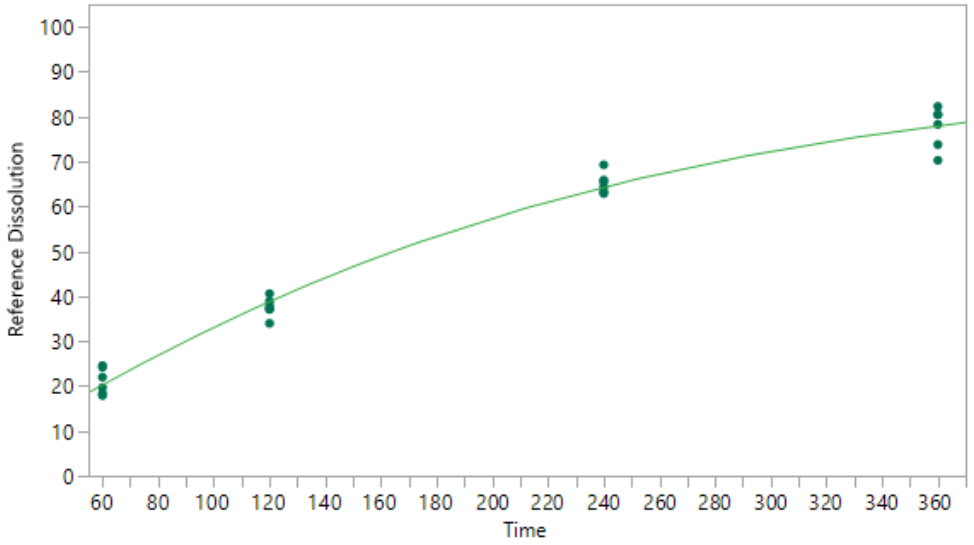


Information quality: what is the goal?

1. Data resolution
2. Data structure
3. Data integration
4. Temporal relevance
5. Chronology of data and goal
6. Generalizability
7. Operationalization
8. Communication

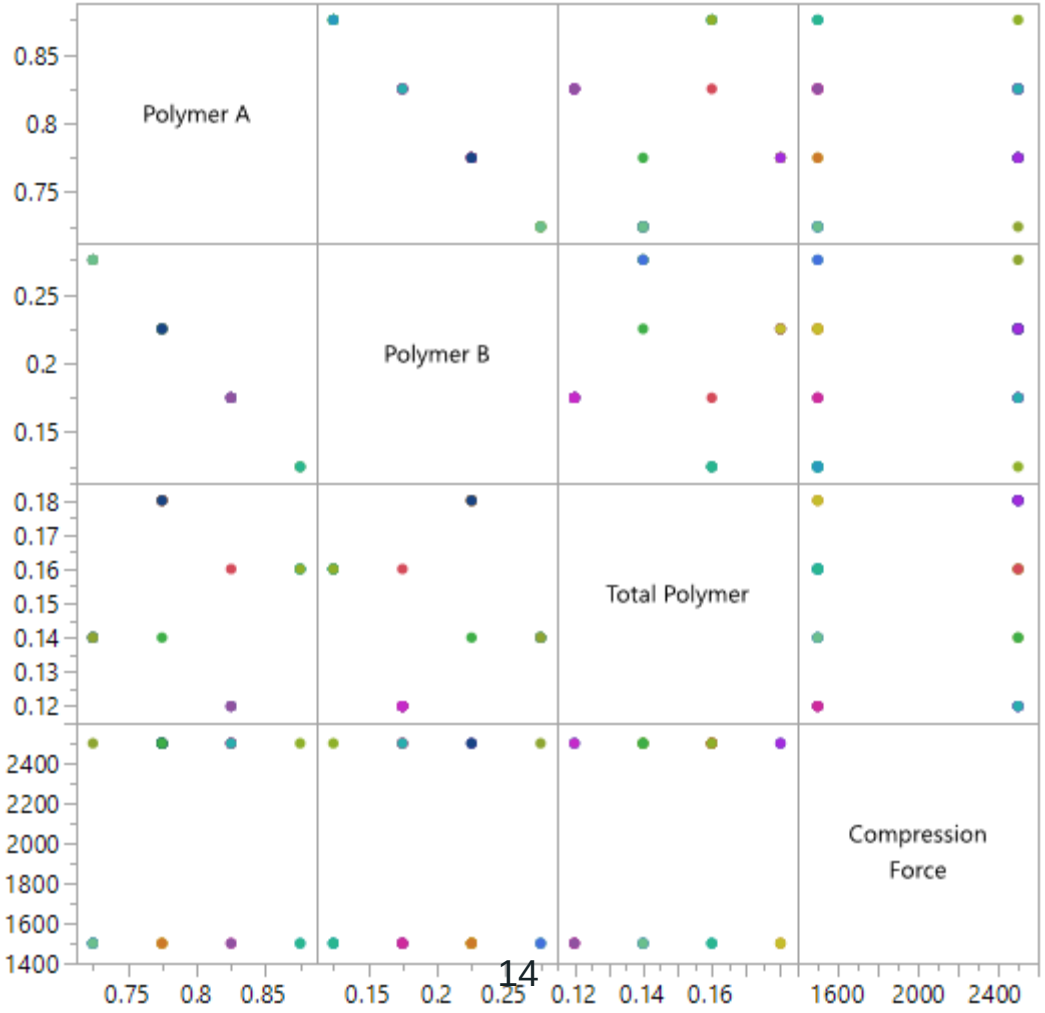


"After all, it is all about information quality….."



Goal: Find Polymer & Compression Values leading to closest match to reference dissolution curve

Factors:
Polymer A (Mixture)
Polymer B (Mixture)
Total Polymer
Compression Force



	Set	Batch	Rep	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60	Dissolution 120	Dissolution 240	Dissolution 360
1	R	R01	1	•	•	•	•	19.7	37.2	63.3	73.8
2	R	R01	2	•	•	•	•	24.2	34.0	64.4	70.3
3	R	R01	3	•	•	•	•	22.0	37.1	65.5	80.5
4	R	R01	4	•	•	•	•	18.4	40.6	62.9	78.3
5	R	R01	5	•	•	•	•	17.9	38.9	65.9	82.3
6	R	R01	6	•	•	•	•	24.6	37.8	69.3	80.5
7	A	A01	1	0.825	0.175	0.16	2500	17.0	26.7	39.6	54.6
8	A	A01	2	0.825	0.175	0.16	2500	22.3	25.9	44.8	57.5
9	A	A01	3	0.825	0.175	0.16	2500	12.7	28.5	45.1	52.9
10	A	A01	4	0.825	0.175	0.16	2500	18.7	28.0	43.9	52.5
11	A	A01	5	0.825	0.175	0.16	2500	19.0	25.8	44.0	54.3
12	A	A01	6	0.825	0.175	0.16	2500	16.1	28.8	44.1	58.0
13	A	A02	1	0.775	0.225	0.14	2500	19.1	36.5	59.9	73.5
14	A	A02	2	0.775	0.225	0.14	2500	18.4	36.1	58.9	75.0
15	A	A02	3	0.775	0.225	0.14	2500	19.3	40.1	59.6	74.6
16	A	A02	4	0.775	0.225	0.14	2500	29.6	38.6	62.7	78.8
17	A	A02	5	0.775	0.225	0.14	2500	19.7	35.2	58.5	73.3
18	A	A02	6	0.775	0.225	0.14	2500	25.2	39.9	62.6	73.8

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3	R	R01	3	•	•	•	•	22.0	37.1	65.5	80.5
4	R	R01	4	•	•	•	•	18.4	40.6	62.9	78.3
5	R	R01	5	•	•	•	•	17.9	38.9	65.9	82.3
6	R	R01	6	•	•	•	•	24.6	37.8	69.3	80.5
7	A	A01	1	0.825	0.175	0.16	2500	17.0	26.7	39.6	54.6
8	A	A01	2	0.825	0.17				25.9	44.8	57.5
9	A	A01	3	0.825	0.17				28.5	45.1	52.9
10	A	A01	4	0.825	0.175	0.16	2500	18.7	28.0	43.9	52.5
11	A	A01	5	0.825	0.175	0.16	2500	19.0	25.8	44.0	54.3
12	A	A01	6	0.825	0.175	0.16	2500	16.1	28.8	44.1	58.0
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14	A	A02	2	0.775	0.225	0.14	2500	18.4	36.1	58.9	75.0
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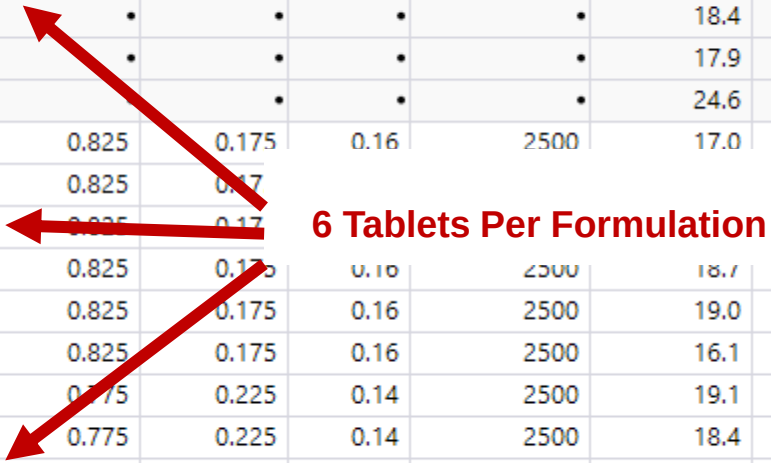
16	A	A02	4	0.775	0.225	0.14	2500	29.6	38.6	62.7	78.8
17	A	A02	5	0.775	0.225	0.14	2500	19.7	35.2	58.5	73.3
18	A	A02	6	0.775	0.225	0.14	2500	25.2	39.9	62.6	73.8



6 Tablets Per Formulation

	Set	Batch	Rep	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60	Dissolution 120	Dissolution 240	Dissolution 360
1	R	R01	1	•	•	•	•	19.7	37.2	63.3	73.8
2	R	R01	2	•	•	•	•	2[illegible]	34.0	64.4	70.3
3	R	R01	3	•	•	•	•	22.0	37.1	65.5	80.5
4	R	R01	4	•	•	•	•	18.4	40.6	62.9	78.3
5	R	R01	5	•	•	•	•	17.9	38.9	65.9	82.3
6	R	R01	6	•	•	•	•	24.6	37.8	69.3	80.5
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11	A	A01	5	0.825	0.175	0.16	2500				
12	A	A01	6	0.825	0.175	0.16	2500				
13	A	A02	1	0.775	0.225	0.14	2500	19.1	36.5	59.9	73.5
14	A	A02	2	0.775	0.225	0.14	2500	18.4	36.1	58.9	75.0
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18	A	A02	6	0.775	0.225	0.14	2500	25.2	39.9	62.6	73.8

4 Dissolution Measurements Per Tablet

	Set	Batch	Rep	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60	Dissolution 120	Dissolution 240	Dissolution 360
1	R	R01	1	•	•	•	•	19.7	37.2	63.3	73.8
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5	R	R01	5	•	•	•	•	17.9	38.9	65.9	82.3
6	R	R01	6	•	•	•	•	24.6	37.8	69.3	80.5
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10	A	A01	4	0.825	0.175	0.16	2500	18.7	28.0	43.9	52.5
11	A	A01	5	0.825	0.175					44.0	54.3
12	A	A01	6	0.825	0.175					44.1	58.0
13	A	A02	1	0.775	0.225	0.14	2500	19.1	36.5	59.9	73.5
14	A	A02	2	0.775	0.225	0.14	2500	18.4	36.1	58.9	75.0
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16 DoE Formulations

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3	R	R01	3	•	•					65.5	80.5
4	R	R01	4	•	•					62.9	78.3
5	R	R01	5	•	•					65.9	82.3
6	R	R01	6	•	•	•	•	24.6	37.8	69.3	80.5
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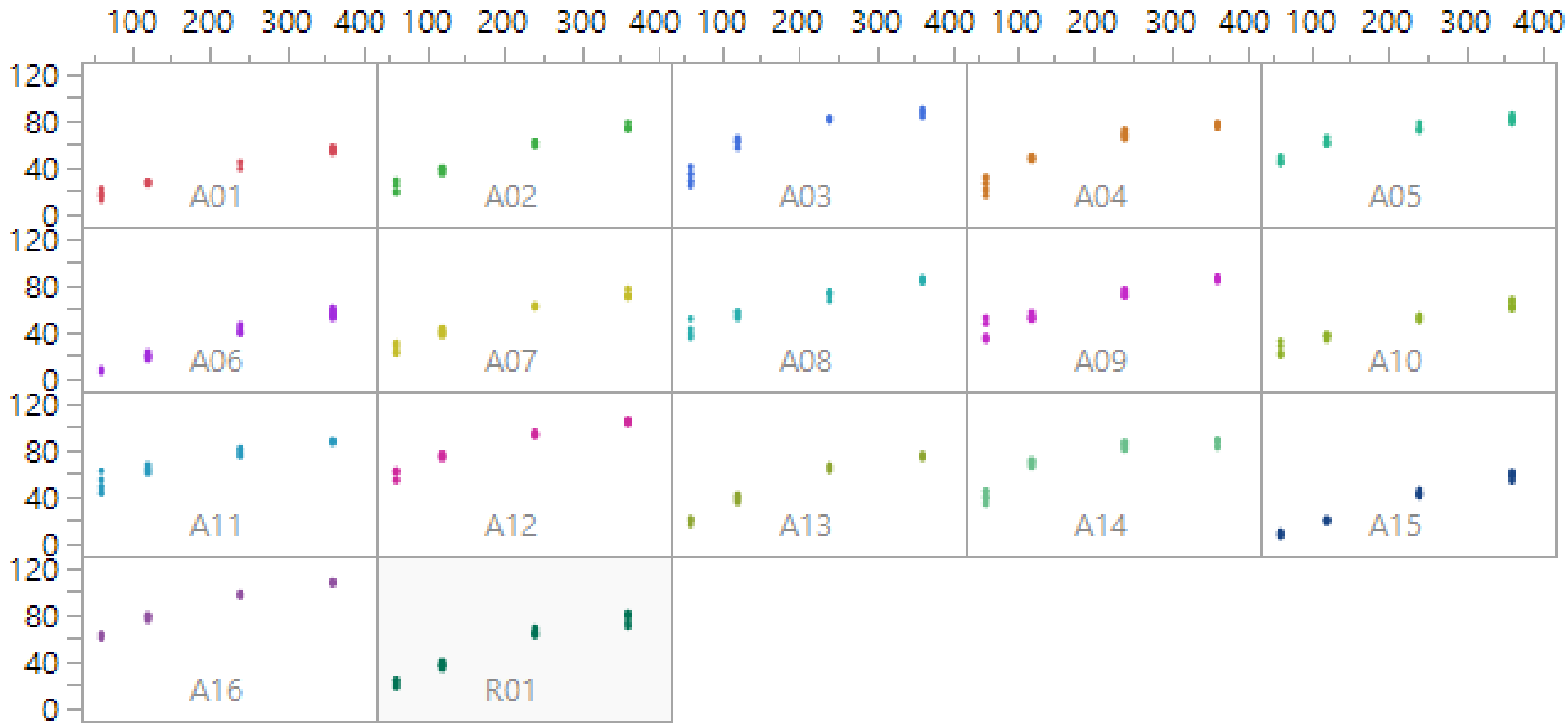


Data Resolution

1) Is the data scale used aligned with the stated goal? *Yes*

2) How reliable and precise are the measuring devices or data sources? *Yes*

3) Is the data analysis suitable for the data aggregation level? *yes, but…*

Data Structure

1) Is the type of the data used aligned with the stated goal? *Clearly yes*

2) Are data integrity details (corrupted/missing values) described and handled appropriately? *N/A (Yes)*

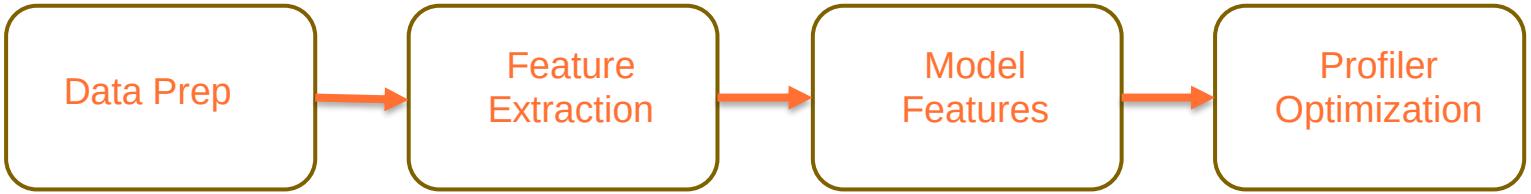
3) Are the analysis methods suitable for the data structure? *Yes, but…*

Data Integration

1) Are the data integrated from multiple sources? *Yes, mildly* -
   If so, what is the credibility of each source? *N/A*
2) How is the integration done? *Feature extraction/Dimension reduction*
3) Are there linkage issues that lead to dropping crucial information? *TBD*
4) Does the data integration add value in terms of the stated goal? *TBD*
5) Does the data integration cause any privacy or confidentiality concerns? *No*

Three Analyses (f2, FDA, NLR)

$$InfoQ(U,f,X,g) = U(f(X|g))$$



Three Analyses (f2, FDA, NLR)

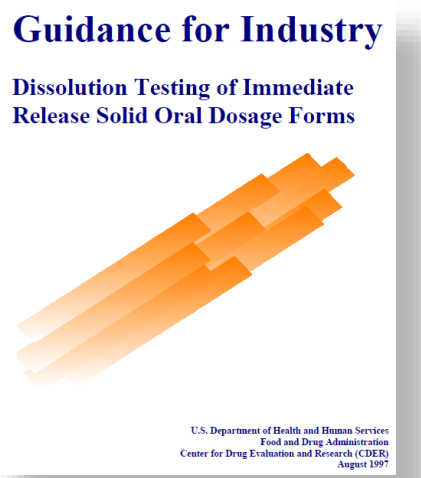
1) **f2 -** Extract f2 scores and model them (GenReg)

2) **FDA -** Functional DoE: Extracted FPC scores (Functional Data Explorer, GenReg)

3) **NLR -** Curve DoE: Extract Weibull Growth parameters (Fit Curve, GenReg)

f2 DoE Analysis

$$f2 = 50 \cdot \log\left(\frac{100}{\sqrt{1+\frac{\sum(\bar{R}_t - T_t)^2}{n}}}\right)$$



R_t = Reference at time t

T_t = Test at time t

$$f2 \geq 50$$

Equivalence Region

f2 DoE Analysis

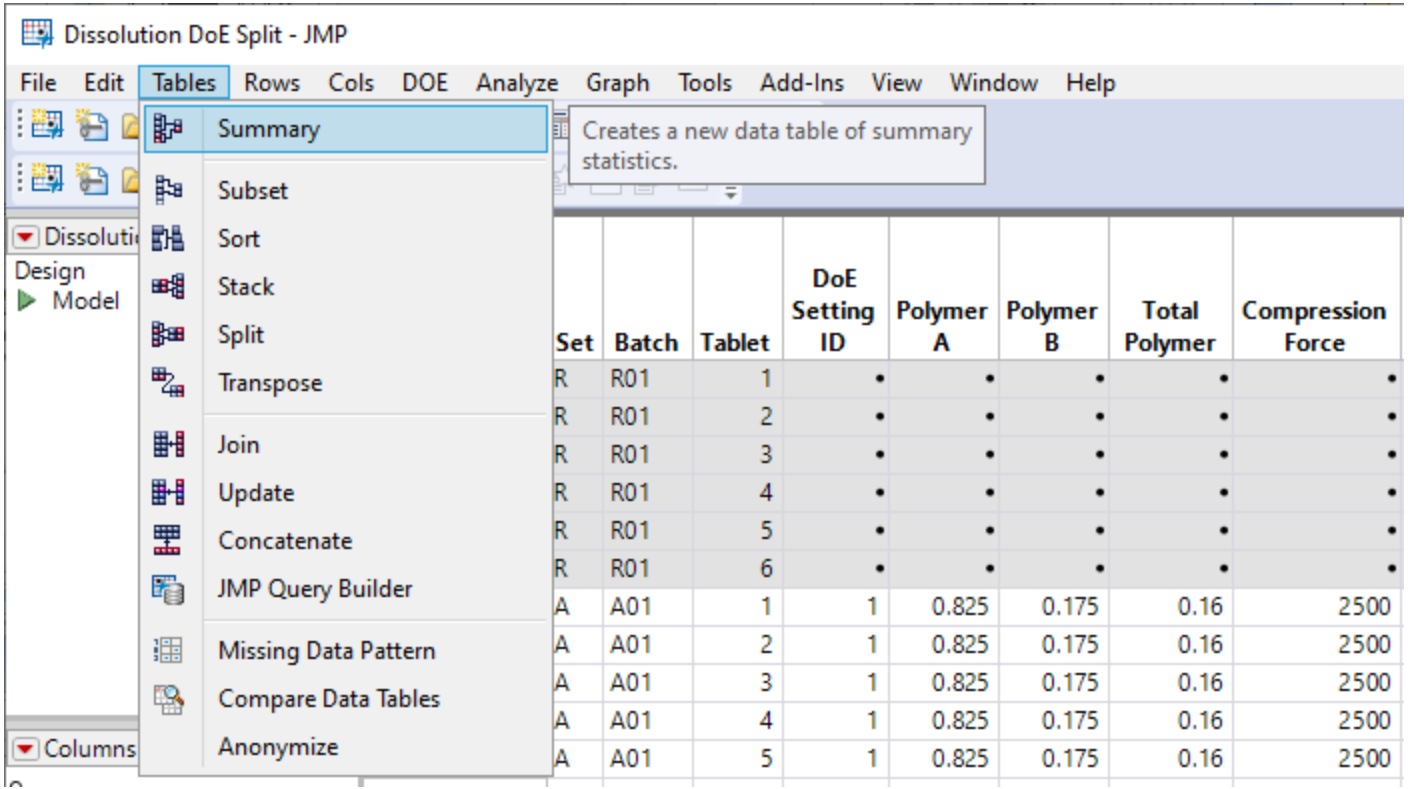
1) Calculate batch means of Dissolution

2) Create a formula column that calculates f2 relative to the reference batch

3) Model f2 using DoE factors as inputs

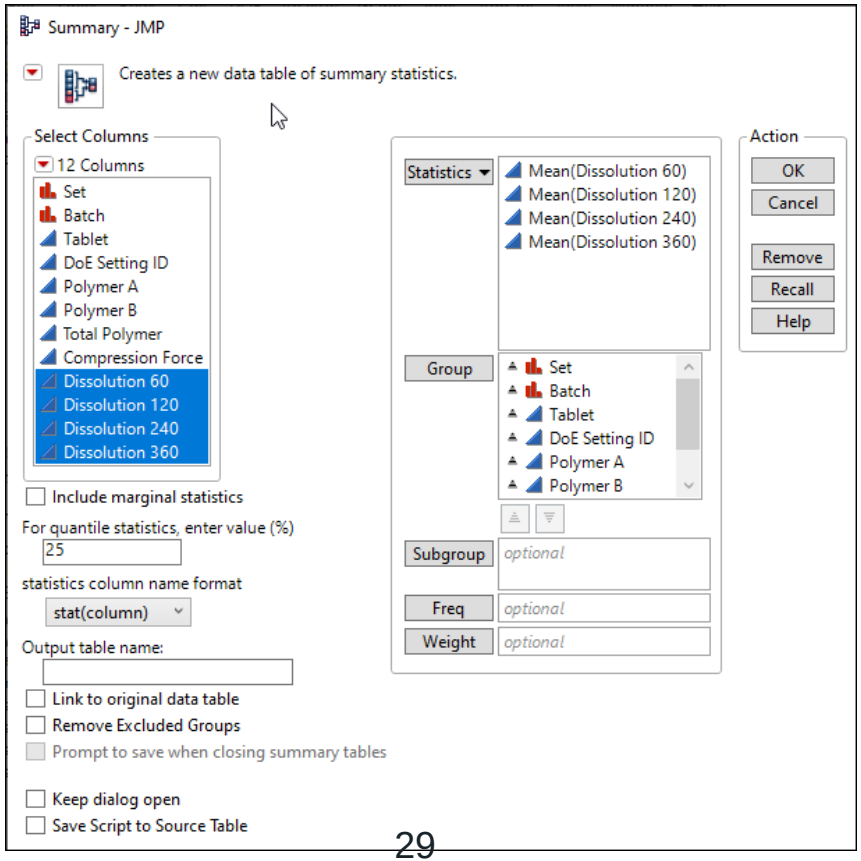
4) Profiler

f2 DoE Analysis

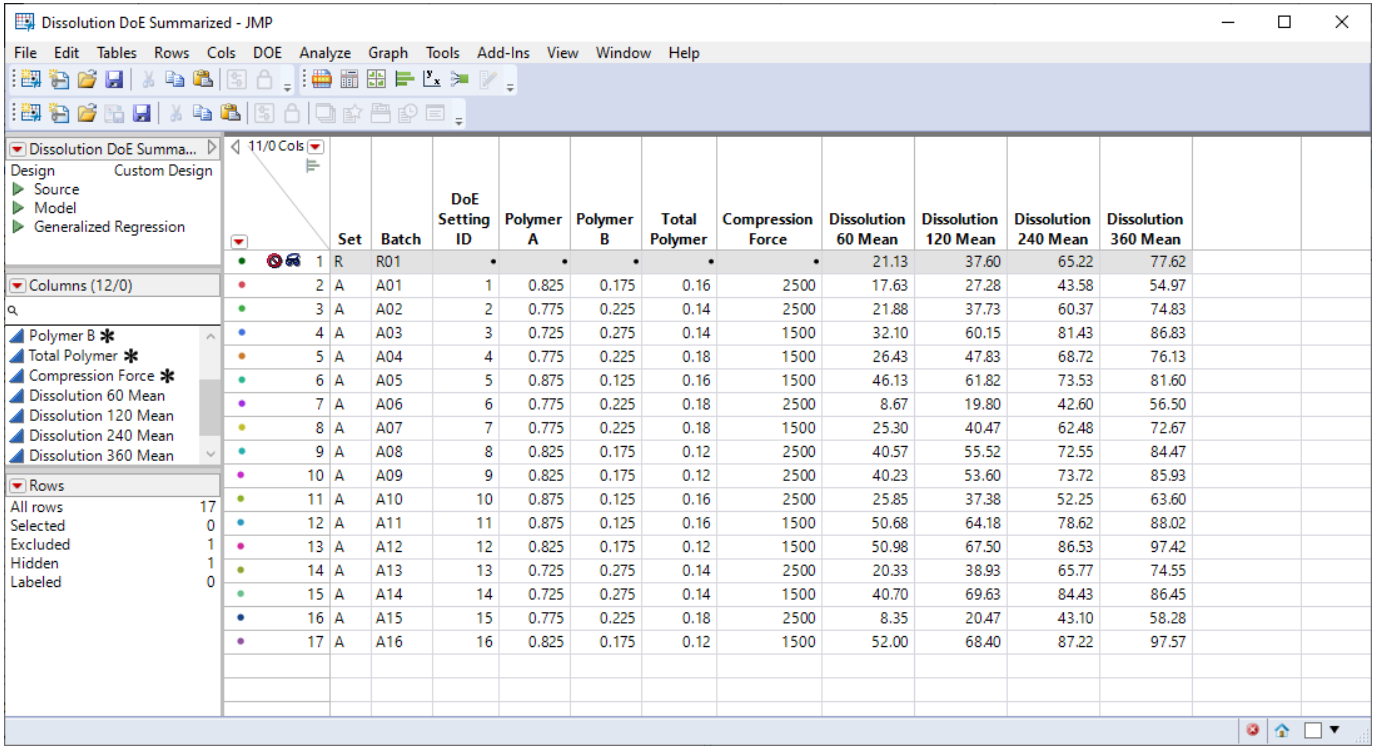


Set	Batch	Tablet	DoE Setting ID	Polymer A	Polymer B	Total Polymer	Compression Force
R	R01	1	•	•	•	•	•
R	R01	2	•	•	•	•	•
R	R01	3	•	•	•	•	•
R	R01	4	•	•	•	•	•
R	R01	5	•	•	•	•	•
R	R01	6	•	•	•	•	•
A	A01	1	1	0.825	0.175	0.16	2500
A	A01	2	1	0.825	0.175	0.16	2500
A	A01	3	1	0.825	0.175	0.16	2500
A	A01	4	1	0.825	0.175	0.16	2500
A	A01	5	1	0.825	0.175	0.16	2500

f2 DoE Analysis



f2 DoE Analysis

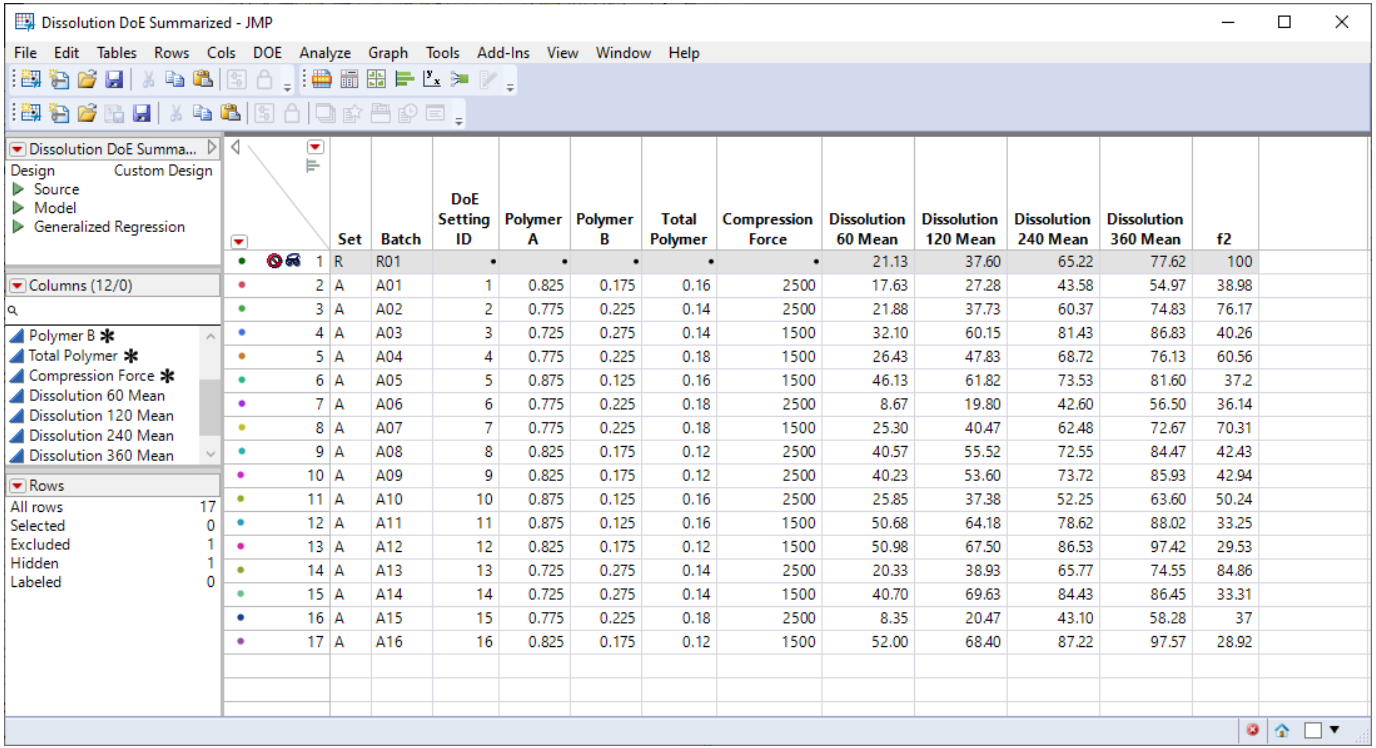


	Set	Batch	DoE Setting ID	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60 Mean	Dissolution 120 Mean	Dissolution 240 Mean	Dissolution 360 Mean
1	R	R01	•	•	•	•	•	21.13	37.60	65.22	77.62
2	A	A01	1	0.825	0.175	0.16	2500	17.63	27.28	43.58	54.97
3	A	A02	2	0.775	0.225	0.14	2500	21.88	37.73	60.37	74.83
4	A	A03	3	0.725	0.275	0.14	1500	32.10	60.15	81.43	86.83
5	A	A04	4	0.775	0.225	0.18	1500	26.43	47.83	68.72	76.13
6	A	A05	5	0.875	0.125	0.16	1500	46.13	61.82	73.53	81.60
7	A	A06	6	0.775	0.225	0.18	2500	8.67	19.80	42.60	56.50
8	A	A07	7	0.775	0.225	0.18	1500	25.30	40.47	62.48	72.67
9	A	A08	8	0.825	0.175	0.12	2500	40.57	55.52	72.55	84.47
10	A	A09	9	0.825	0.175	0.12	2500	40.23	53.60	73.72	85.93
11	A	A10	10	0.875	0.125	0.16	2500	25.85	37.38	52.25	63.60
12	A	A11	11	0.875	0.125	0.16	1500	50.68	64.18	78.62	88.02
13	A	A12	12	0.825	0.175	0.12	1500	50.98	67.50	86.53	97.42
14	A	A13	13	0.725	0.275	0.14	2500	20.33	38.93	65.77	74.55
15	A	A14	14	0.725	0.275	0.14	1500	40.70	69.63	84.43	86.45
16	A	A15	15	0.775	0.225	0.18	2500	8.35	20.47	43.10	58.28
17	A	A16	16	0.825	0.175	0.12	1500	52.00	68.40	87.22	97.57

f2 DoE Analysis

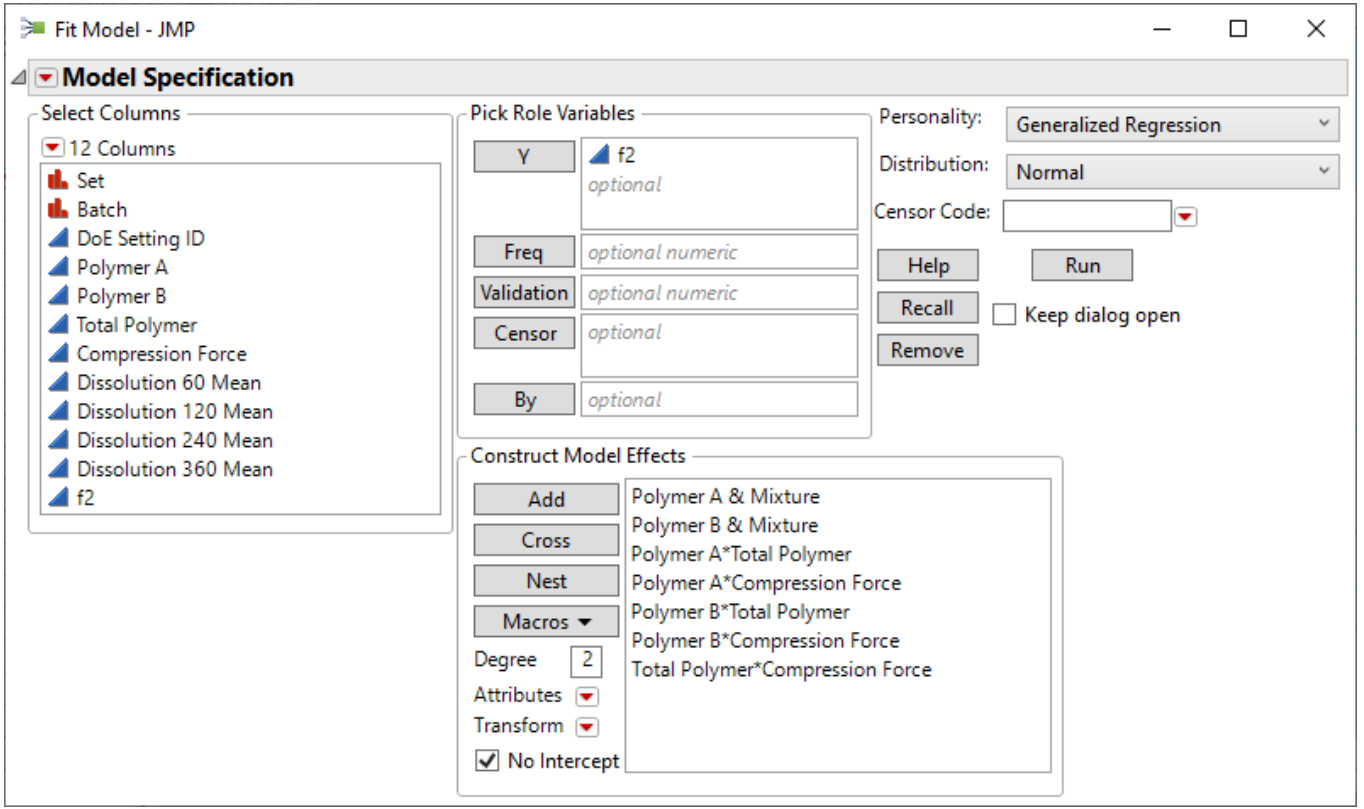
$$50 \cdot \text{Log10}\left(100 \cdot \left(1 + \left(\frac{1}{4}\right) \cdot \left(\begin{array}{l}(\text{Dissolution 60 Mean} - 21.13)^2 \\ + (\text{Dissolution 120 Mean} - 37.6)^2 \\ + (\text{Dissolution 240 Mean} - 65.22)^2 \\ + (\text{Dissolution 360 Mean} - 77.62)^2\end{array}\right)^{-0.5}\right)\right)$$

f2 DoE Analysis

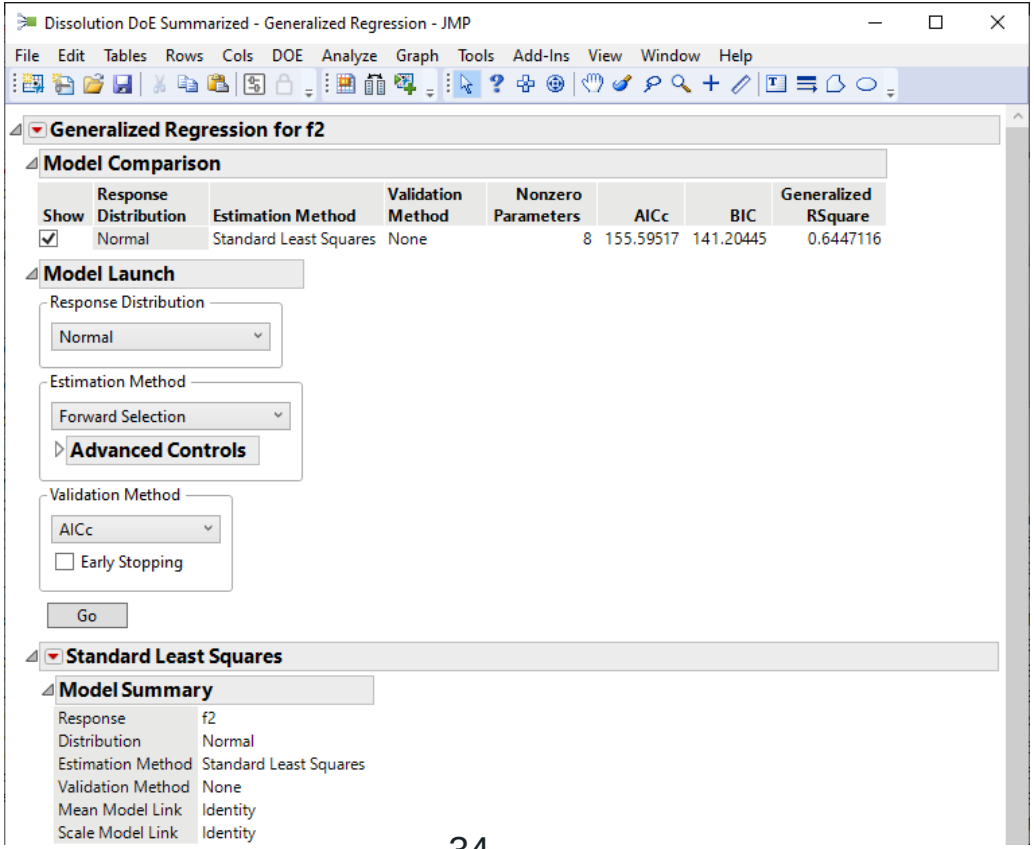


	Set	Batch	DoE Setting ID	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60 Mean	Dissolution 120 Mean	Dissolution 240 Mean	Dissolution 360 Mean	f2
1	R	R01	.	.	.	.	.	21.13	37.60	65.22	77.62	100
2	A	A01	1	0.825	0.175	0.16	2500	17.63	27.28	43.58	54.97	38.98
3	A	A02	2	0.775	0.225	0.14	2500	21.88	37.73	60.37	74.83	76.17
4	A	A03	3	0.725	0.275	0.14	1500	32.10	60.15	81.43	86.83	40.26
5	A	A04	4	0.775	0.225	0.18	1500	26.43	47.83	68.72	76.13	60.56
6	A	A05	5	0.875	0.125	0.16	1500	46.13	61.82	73.53	81.60	37.2
7	A	A06	6	0.775	0.225	0.18	2500	8.67	19.80	42.60	56.50	36.14
8	A	A07	7	0.775	0.225	0.18	1500	25.30	40.47	62.48	72.67	70.31
9	A	A08	8	0.825	0.175	0.12	2500	40.57	55.52	72.55	84.47	42.43
10	A	A09	9	0.825	0.175	0.12	2500	40.23	53.60	73.72	85.93	42.94
11	A	A10	10	0.875	0.125	0.16	2500	25.85	37.38	52.25	63.60	50.24
12	A	A11	11	0.875	0.125	0.16	1500	50.68	64.18	78.62	88.02	33.25
13	A	A12	12	0.825	0.175	0.12	1500	50.98	67.50	86.53	97.42	29.53
14	A	A13	13	0.725	0.275	0.14	2500	20.33	38.93	65.77	74.55	84.86
15	A	A14	14	0.725	0.275	0.14	1500	40.70	69.63	84.43	86.45	33.31
16	A	A15	15	0.775	0.225	0.18	2500	8.35	20.47	43.10	58.28	37
17	A	A16	16	0.825	0.175	0.12	1500	52.00	68.40	87.22	97.57	28.92

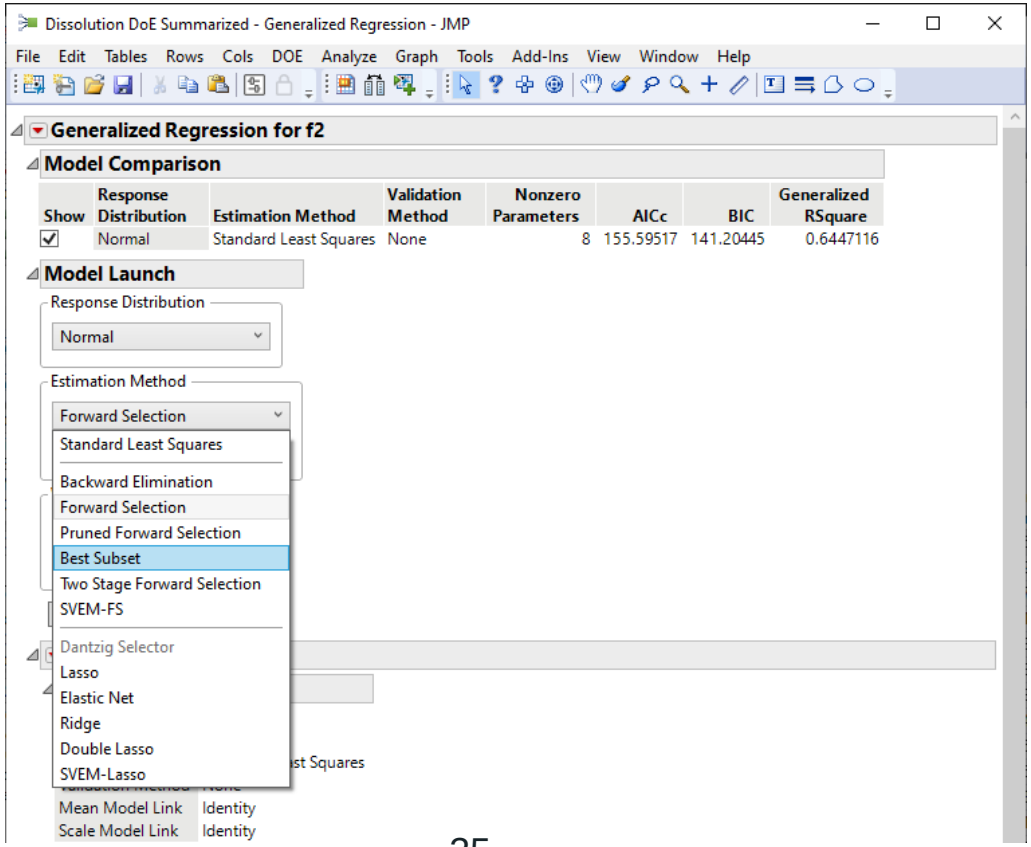
f2 DoE Analysis



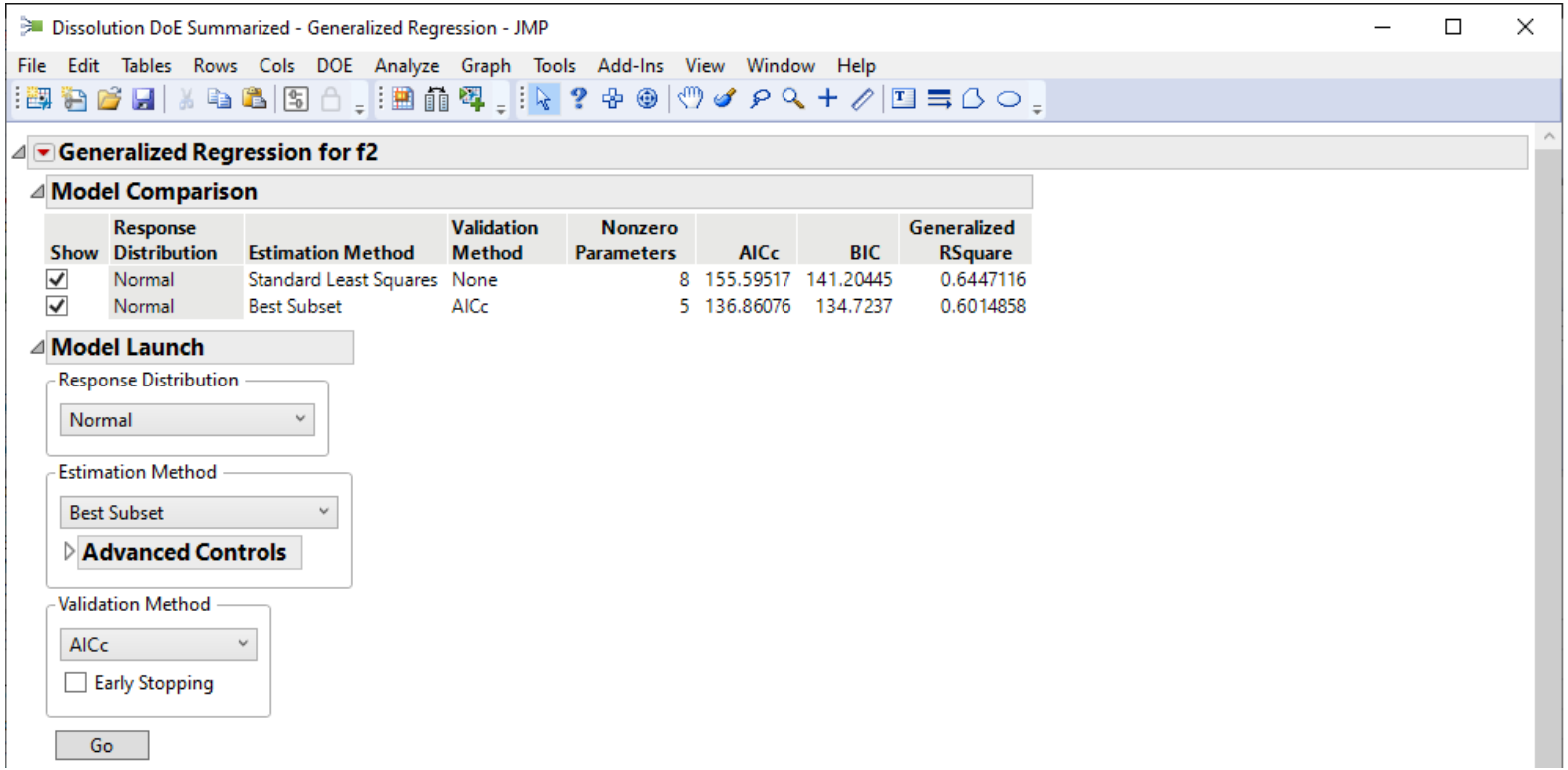
f2 DoE Analysis



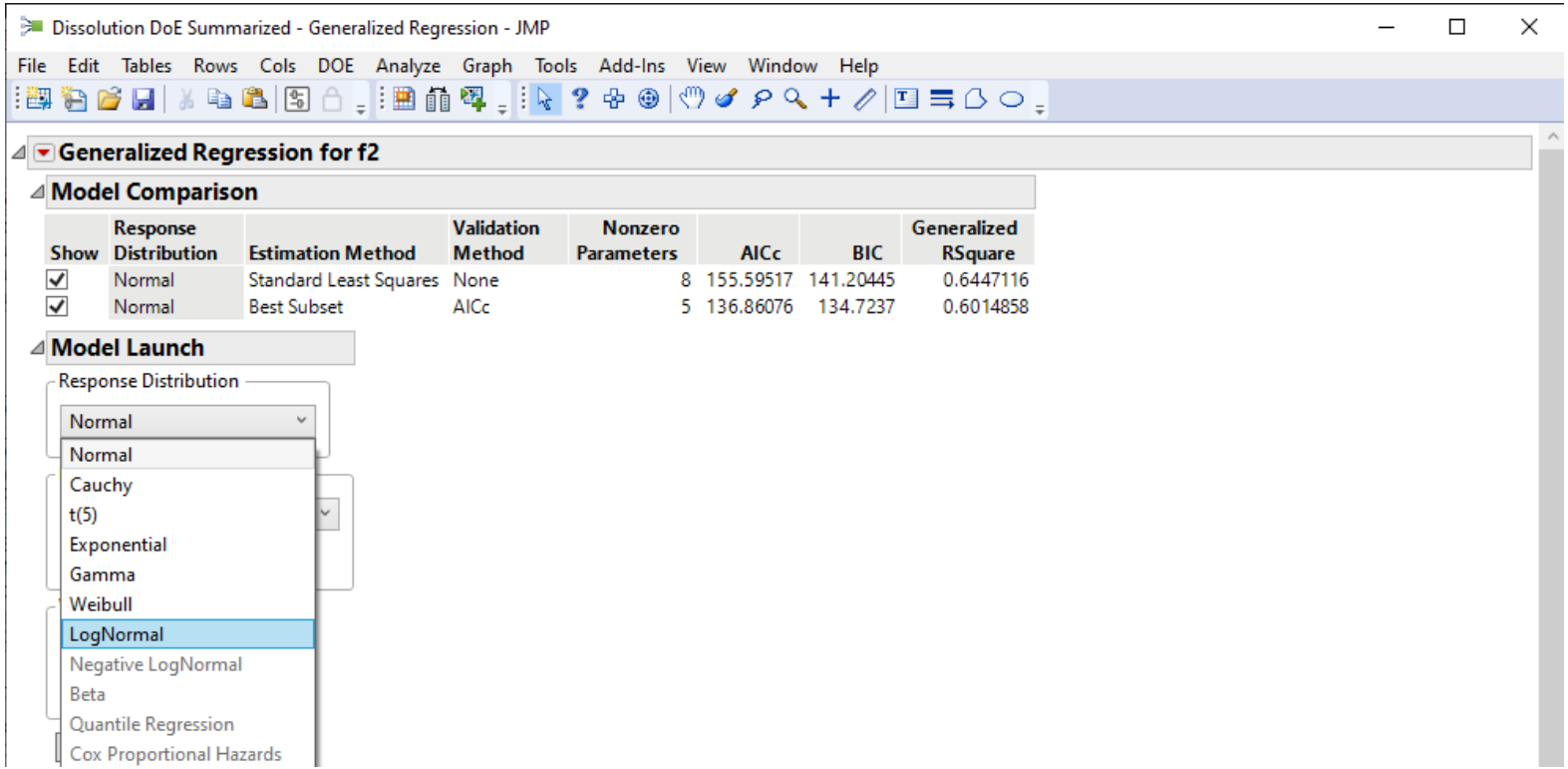
f2 DoE Analysis



f2 DoE Analysis



f2 DoE Analysis



f2 DoE Analysis

Generalized Regression for f2

Model Comparison

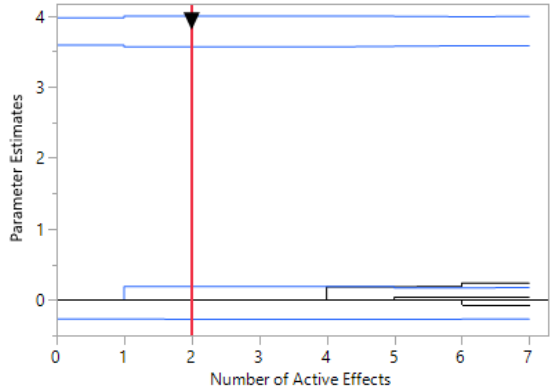
Show	Response Distribution	Estimation Method	Validation Method	Nonzero Parameters	AICc	BIC	Generalized RSquare
☑	Normal	Standard Least Squares	None	8	155.59517	141.20445	0.6447116
☑	Normal	Best Subset	AICc	5	136.86076	134.7237	0.6014858
☑	LogNormal	Best Subset	AICc	5	130.6234	128.48635	0.9972659

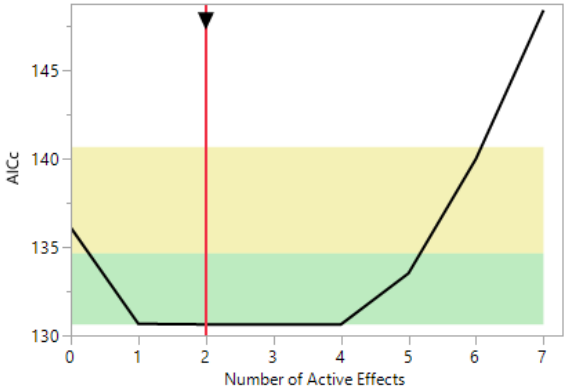
f2 DoE Analysis

LogNormal Best Subset with AICc Validation

Model Summary

Solution Path



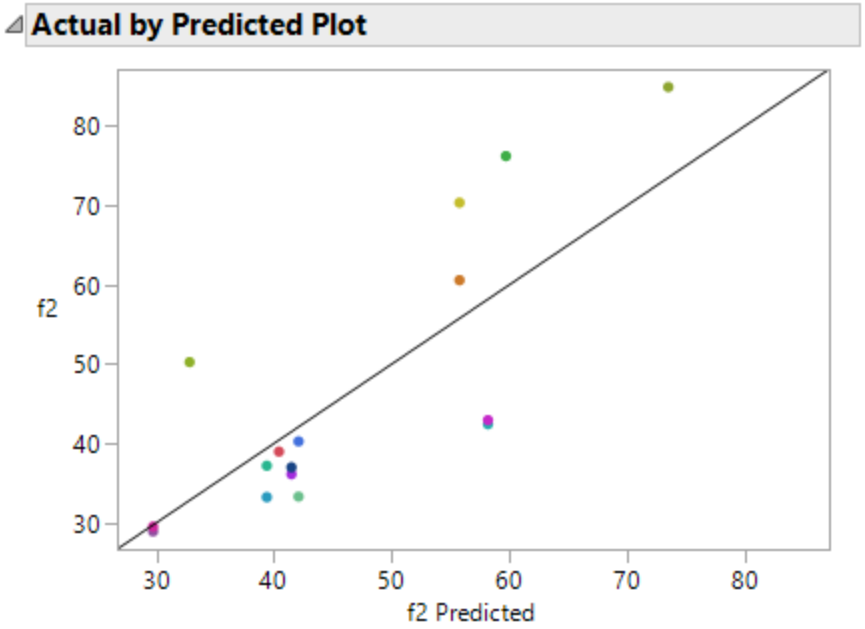


Reset Solution

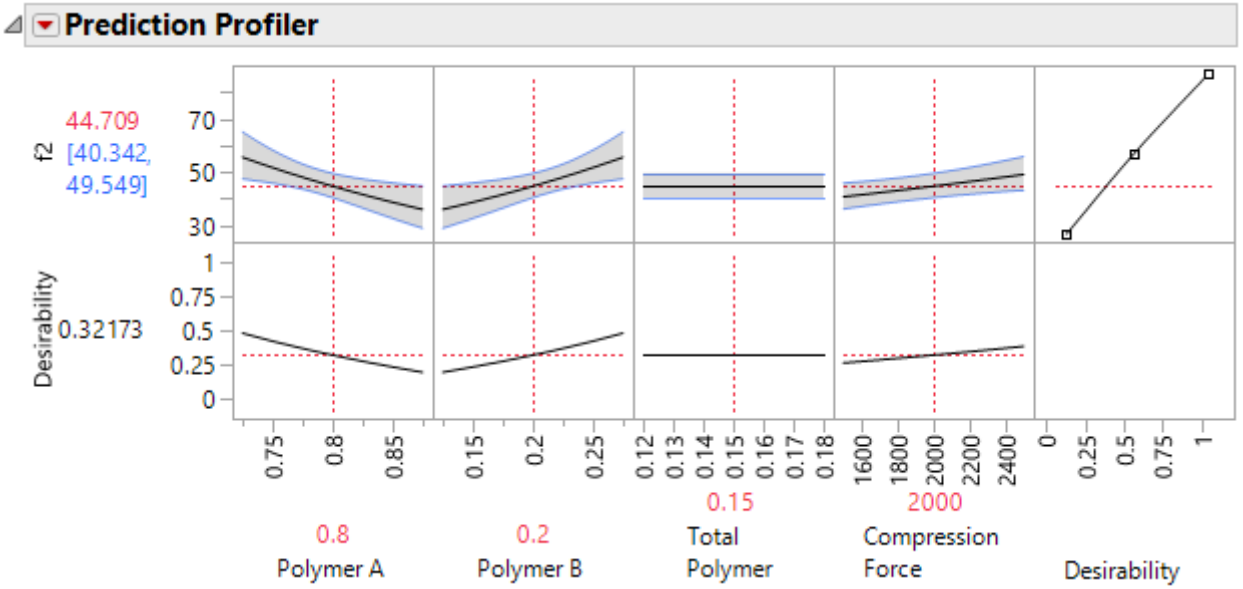
Parameter Estimates for Original Predictors

Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	3.5626664	0.1079872	1088.4423	<.0001*	3.3510153	3.7743176
(Polymer B-0.125)/0.15	Forced in	3.9983247	0.0831121	2314.3406	<.0001*	3.835428	4.1612215
Polymer A*Total Polymer		0	0	0	1.0000	0	0
Polymer A*Compression Force		0	0	0	1.0000	0	0
Polymer B*Total Polymer		0	0	0	1.0000	0	0
Polymer B*Compression Force		0.1876153	0.0718107	6.8258828	0.0090*	0.046869	0.3283616
Total Polymer*Compression Force		-0.272834	0.0632256	18.621392	<.0001*	-0.396754	-0.148914

f2 DoE Analysis



f2 DoE Analysis



f2 DoE Analysis

Functional DoE Analysis (FDA)

Dissolution DoE - JMP

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

Dissolution DoE

Design Custom Design

Model

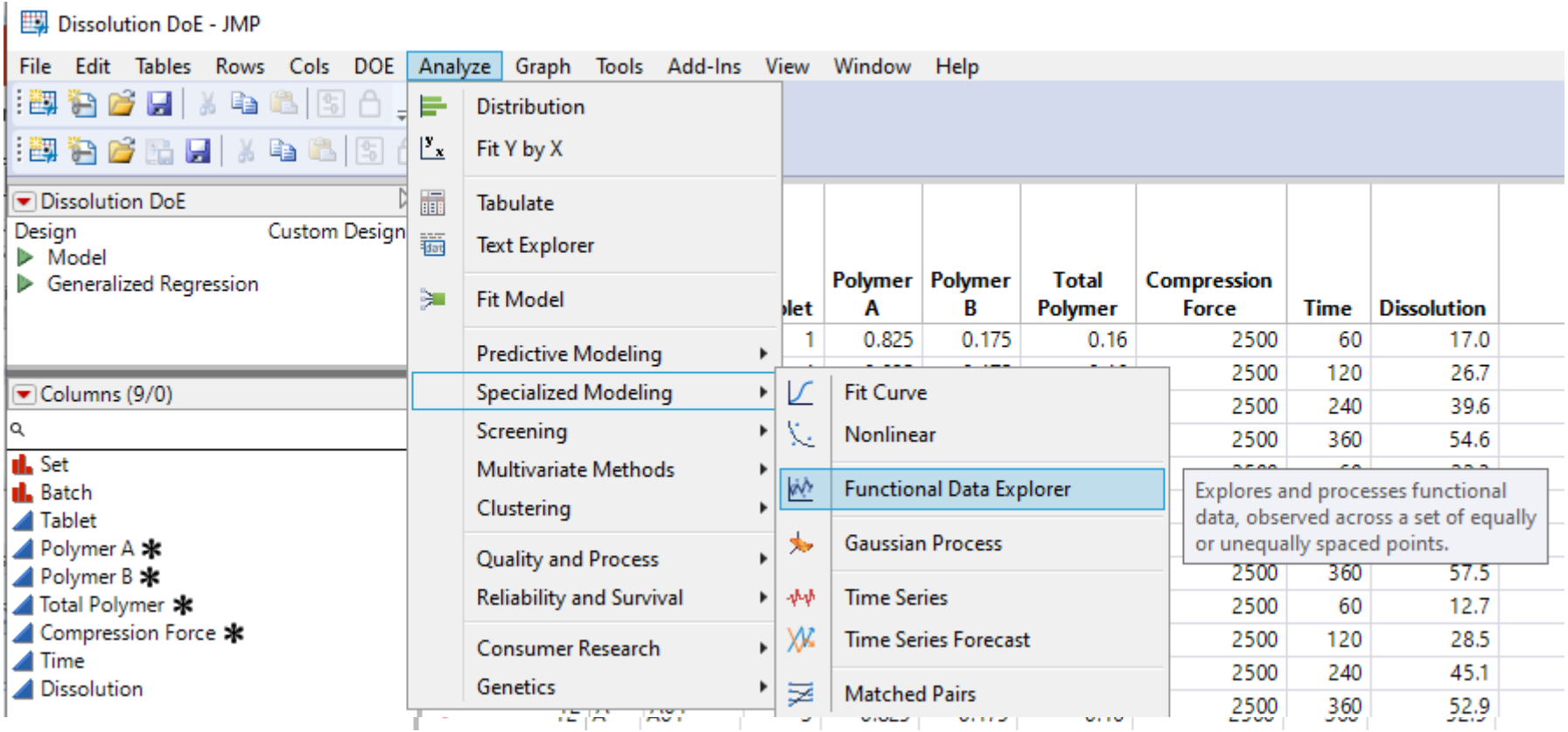
Generalized Regression

Columns (9/0)

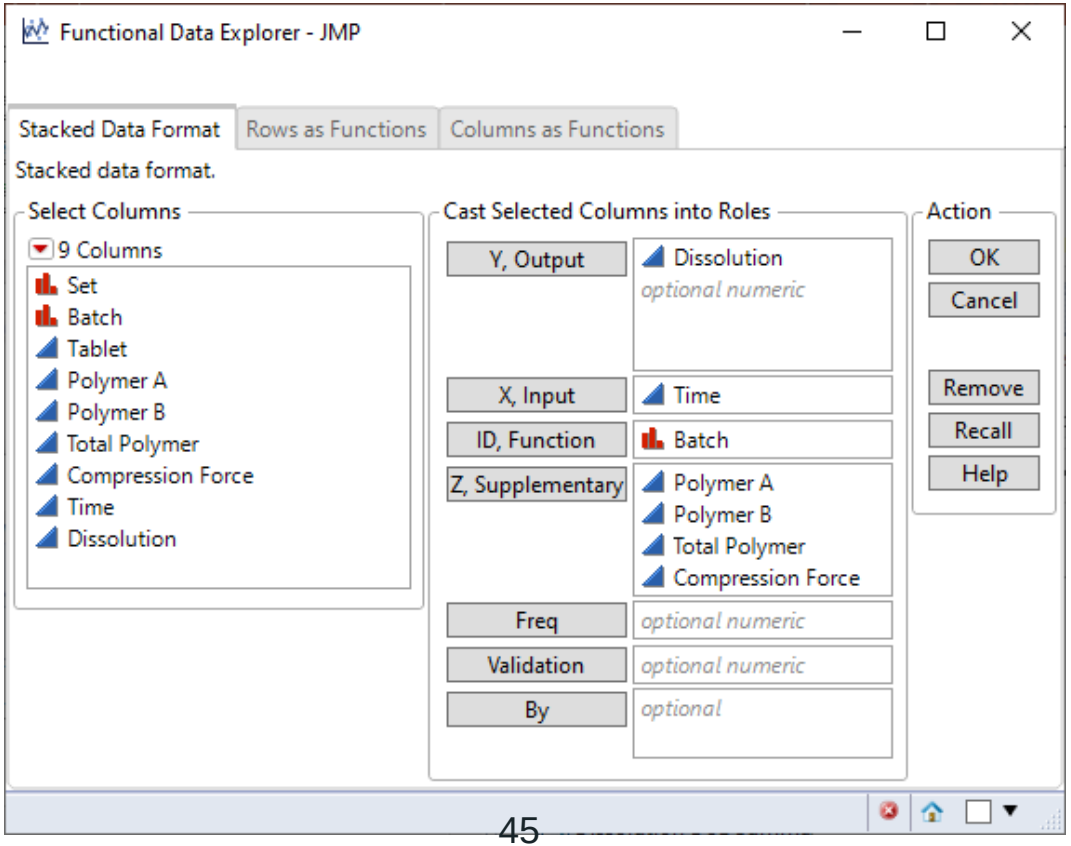
Set
Batch
Tablet
Polymer A *
Polymer B *
Total Polymer *
Compression Force *
Time
Dissolution

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
1	A	A01	1	0.825	0.175	0.16	2500	60	17.0
2	A	A01	1	0.825	0.175	0.16	2500	120	26.7
3	A	A01	1	0.825	0.175	0.16	2500	240	39.6
4	A	A01	1	0.825	0.175	0.16	2500	360	54.6
5	A	A01	2	0.825	0.175	0.16	2500	60	22.3
6	A	A01	2	0.825	0.175	0.16	2500	120	25.9
7	A	A01	2	0.825	0.175	0.16	2500	240	44.8
8	A	A01	2	0.825	0.175	0.16	2500	360	57.5
9	A	A01	3	0.825	0.175	0.16	2500	60	12.7
10	A	A01	3	0.825	0.175	0.16	2500	120	28.5
11	A	A01	3	0.825	0.175	0.16	2500	240	45.1
12	A	A01	3	0.825	0.175	0.16	2500	360	52.9

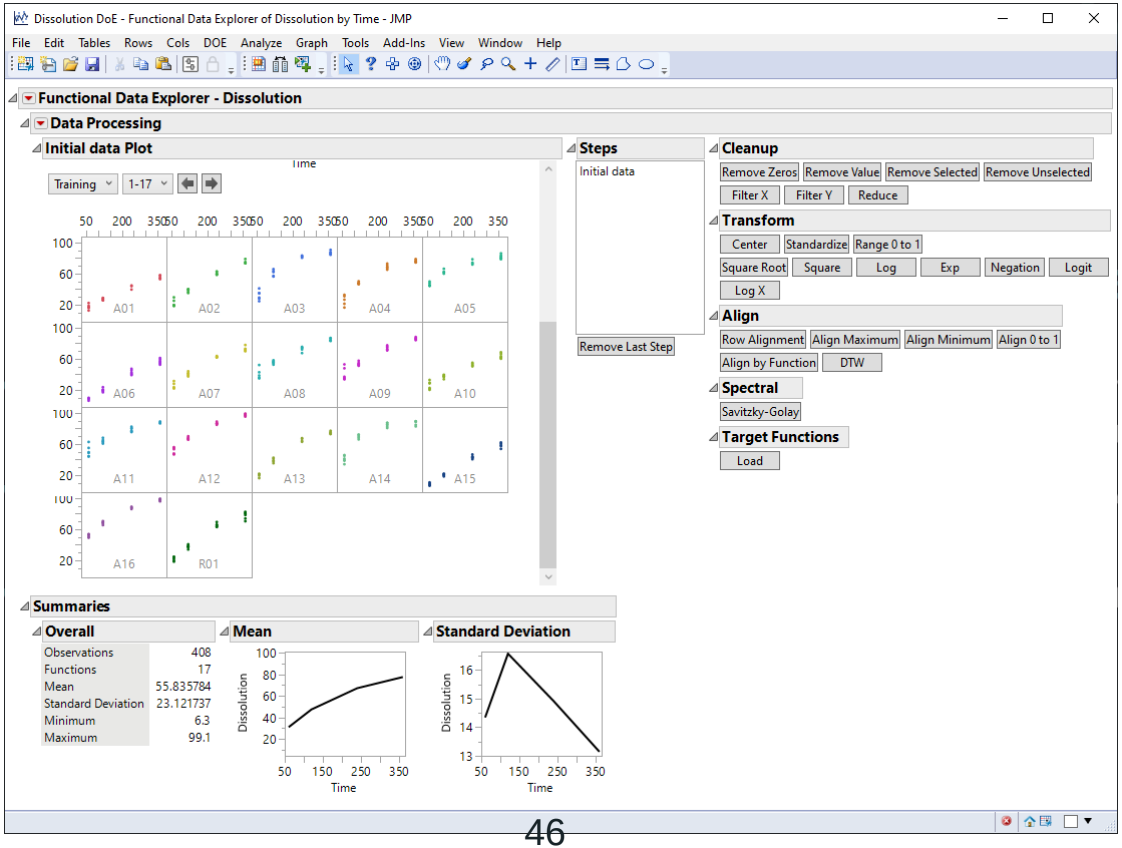
Functional DoE Analysis (FDA)



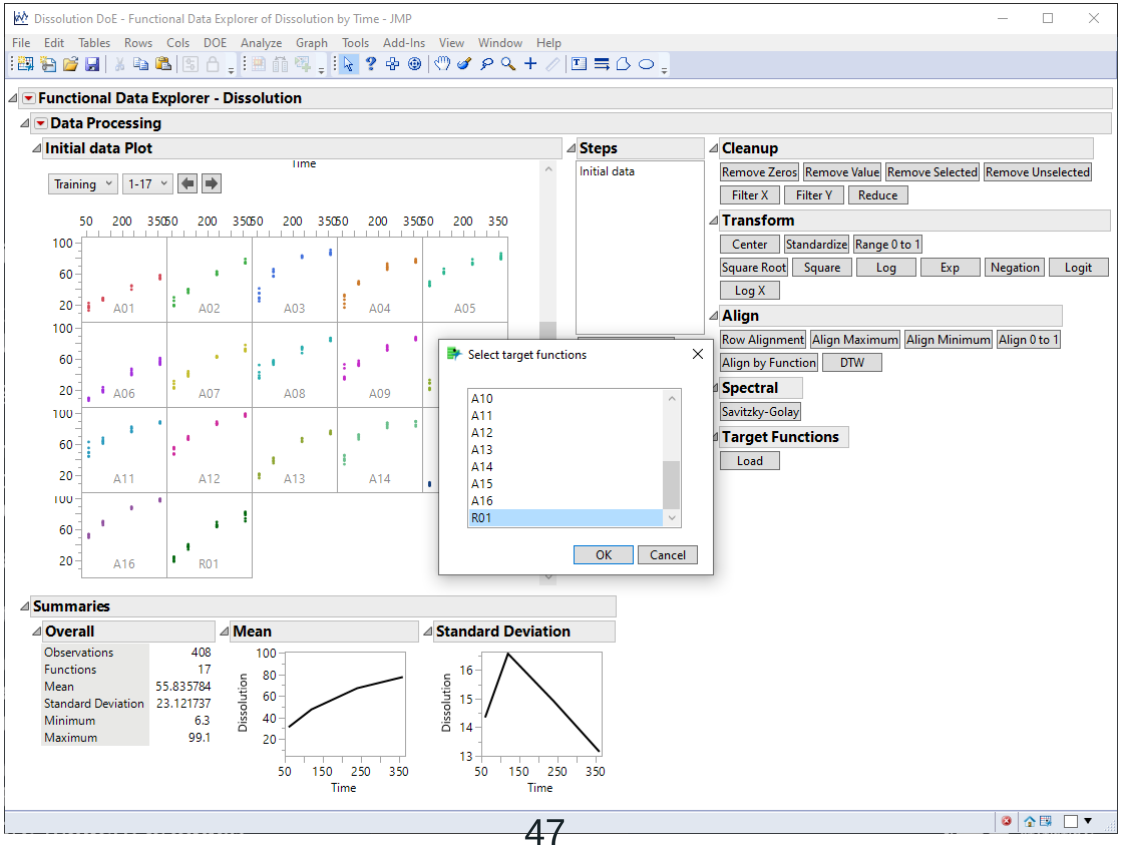
Functional DoE Analysis (FDA)



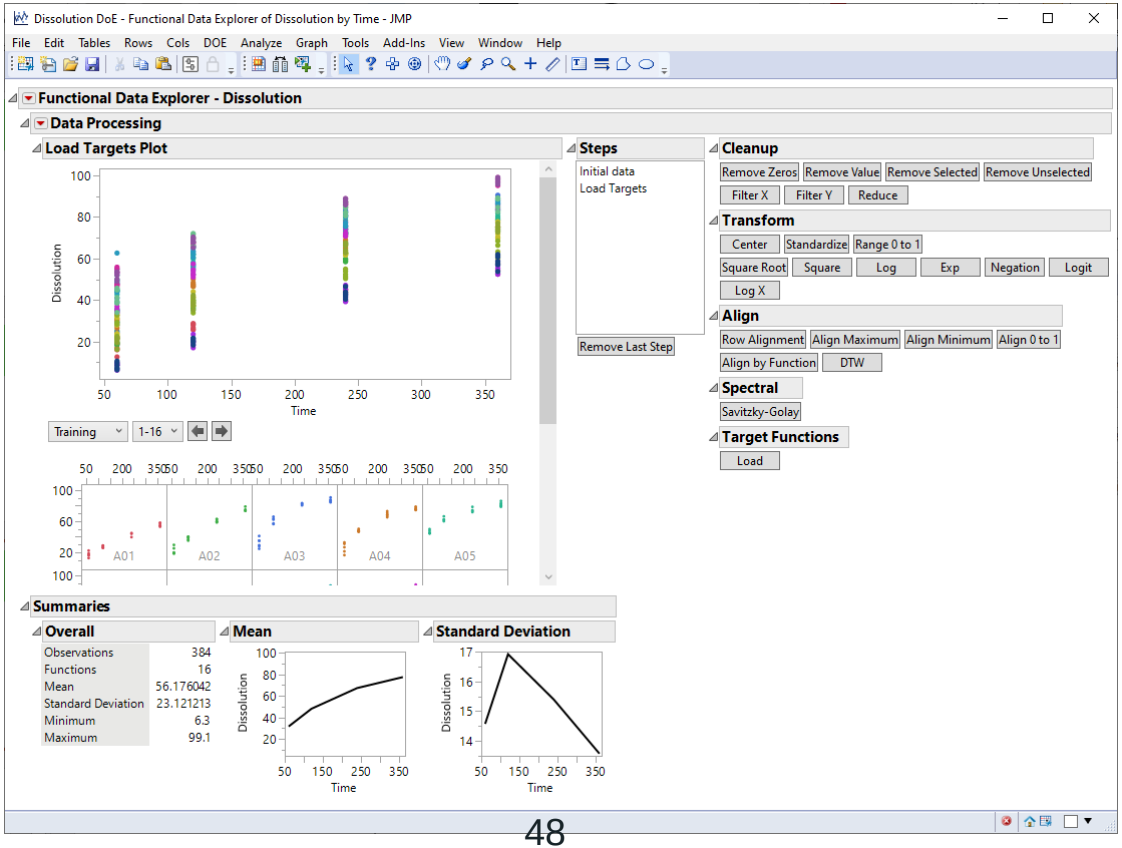
Functional DoE Analysis (FDA)



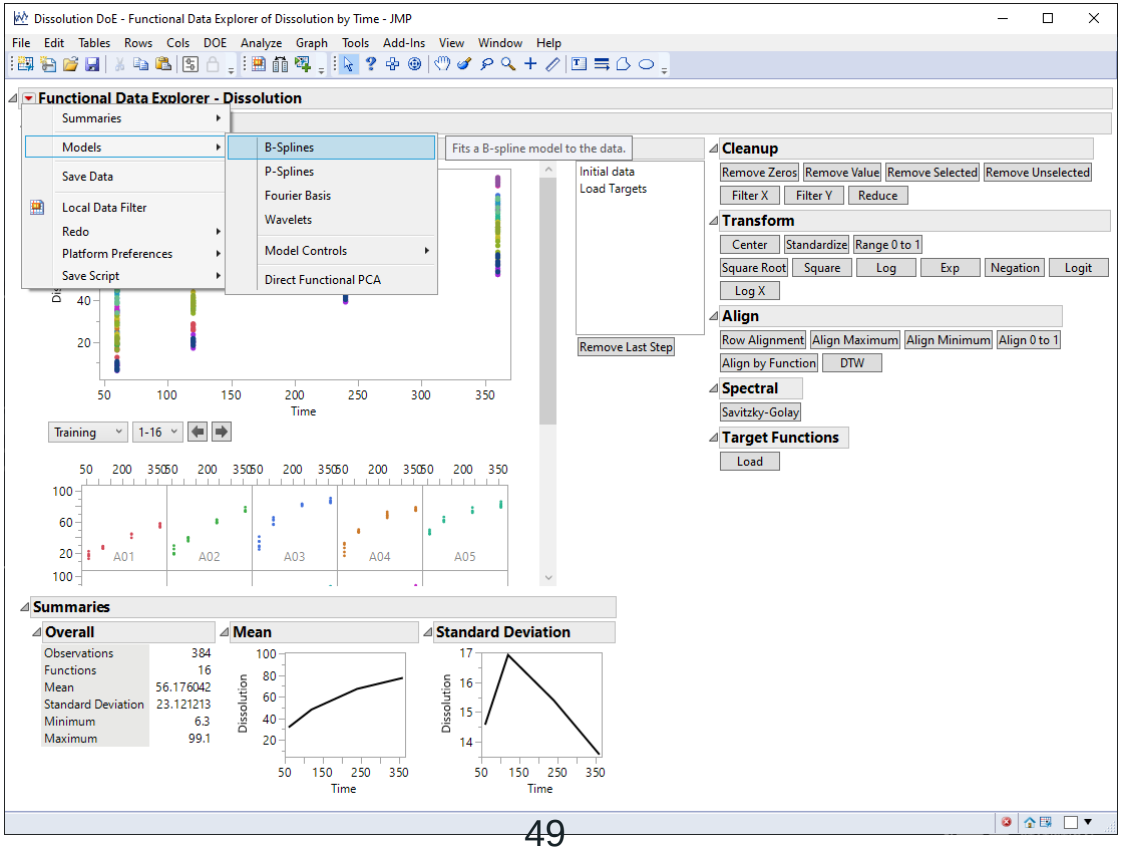
Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)



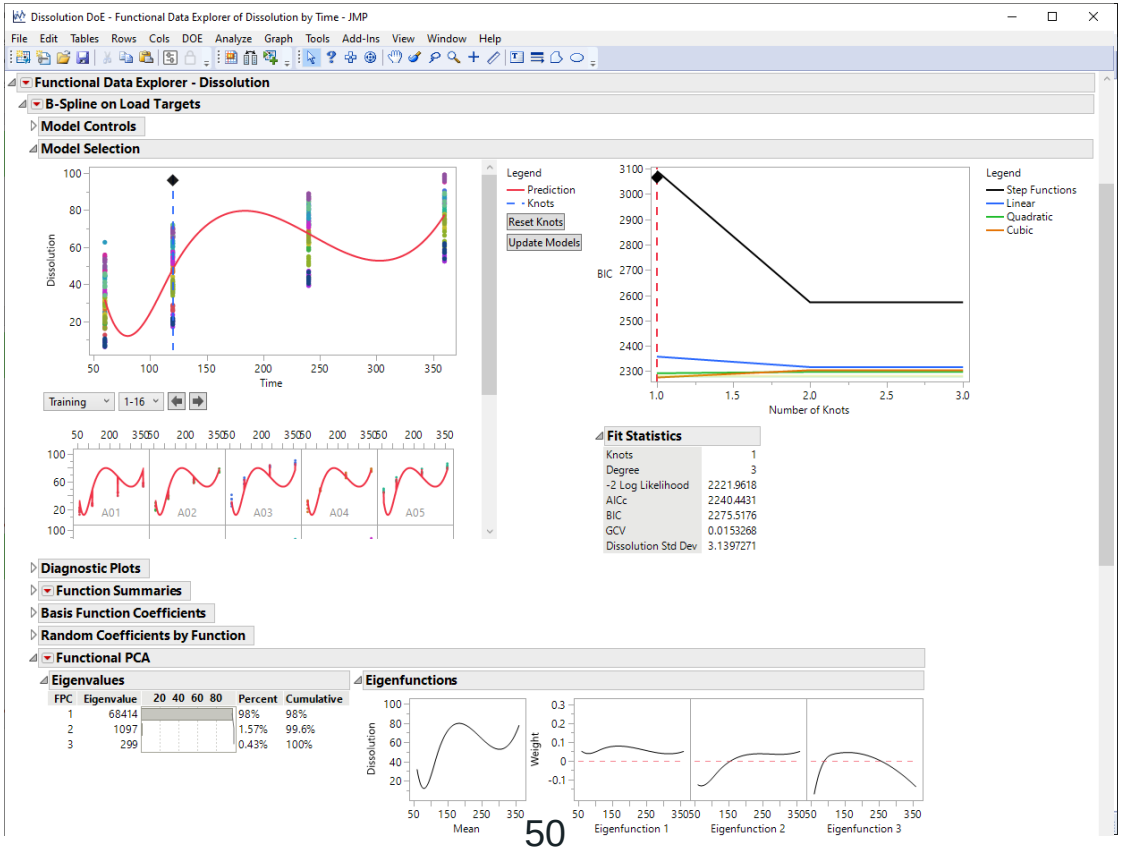
Functional DoE Analysis (FDA)



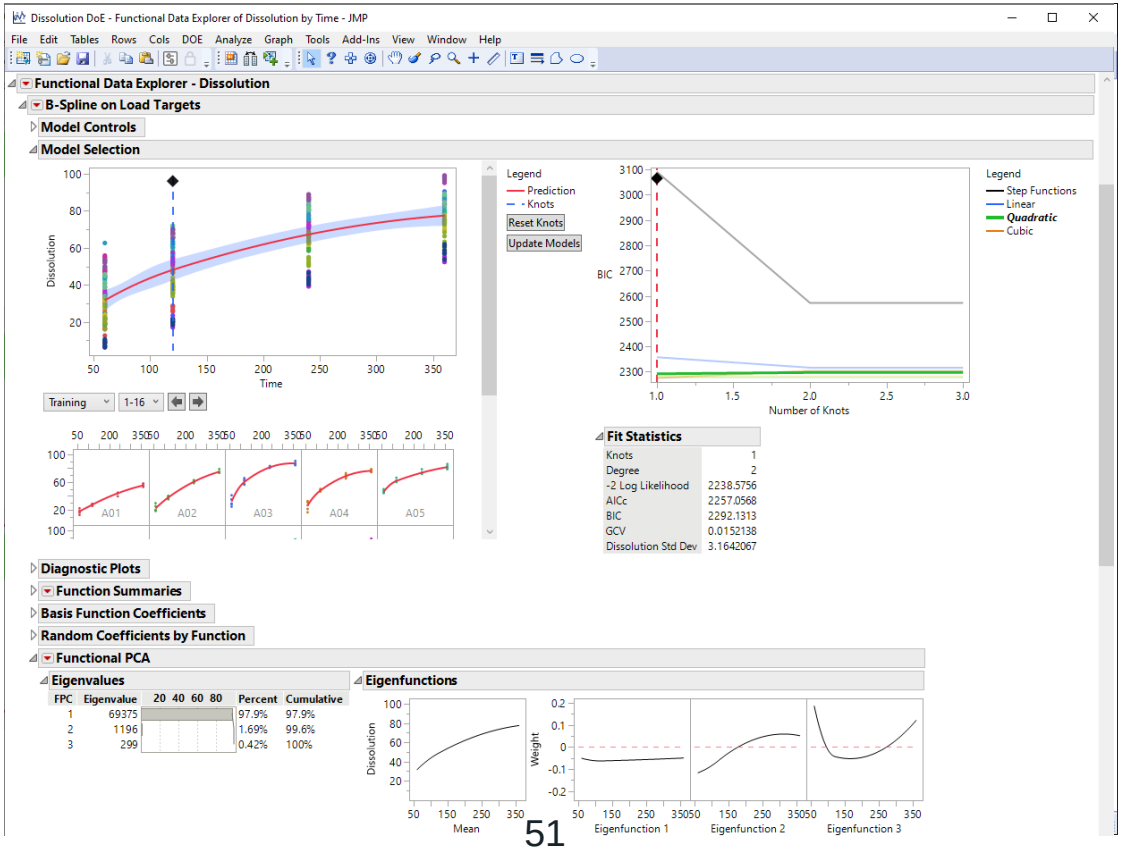
KPA Insights through analytics

jmp STATISTICAL DISCOVERY

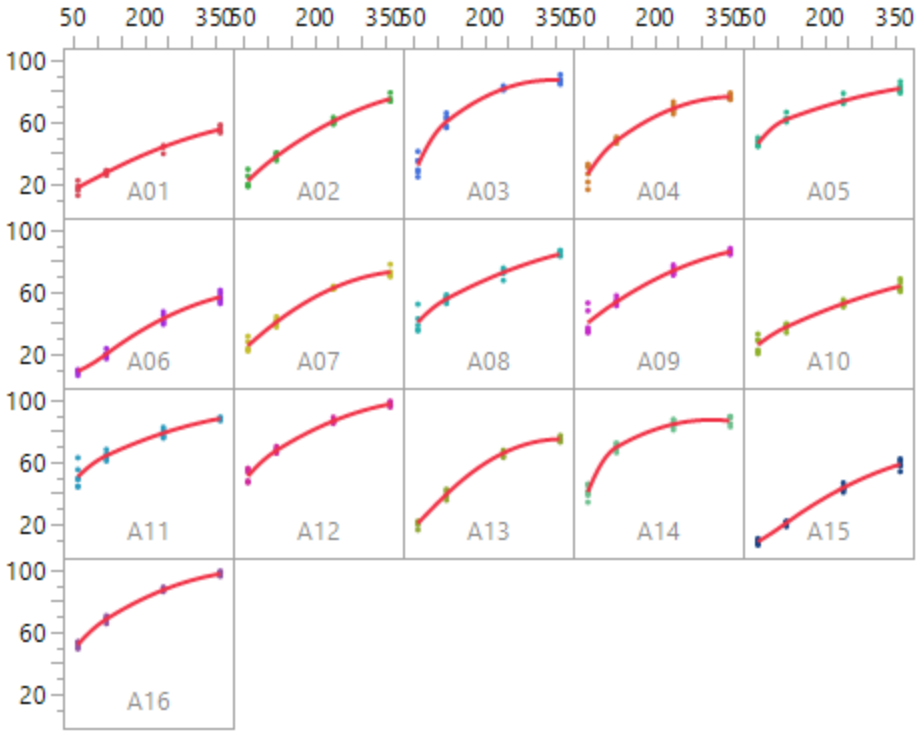
Functional DoE Analysis (FDA)



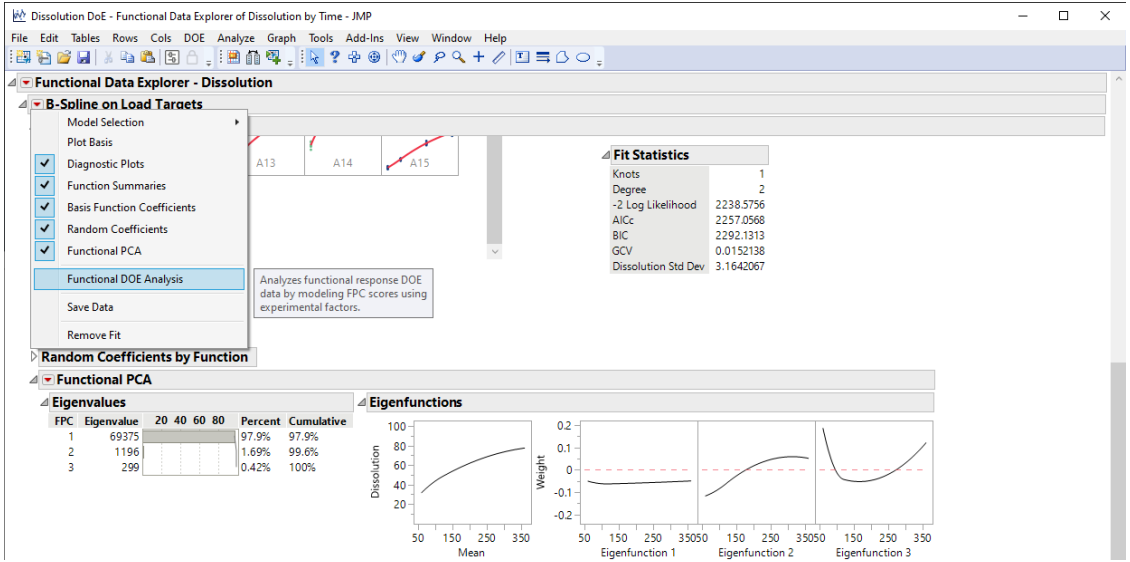
Functional DoE Analysis (FDA)



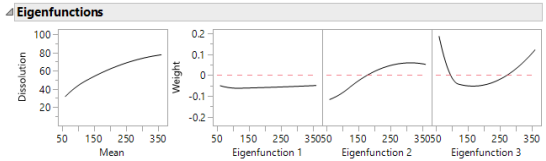
Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)



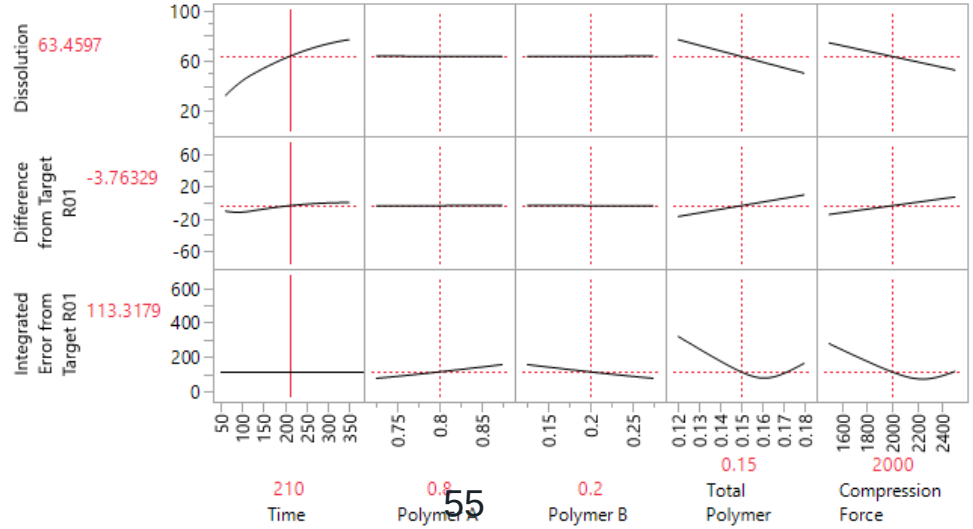
Functional DoE Analysis (FDA)



	Batch	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution FPC 1	Dissolution FPC 2	Dissolution FPC 3
1	A01	0.825	0.175	0.16	2500	377	-48.5	-5.36
2	A02	0.775	0.225	0.14	2500	131.6	32.75	11.98
3	A03	0.725	0.275	0.14	1500	-204	37.78	-26.7
4	A04	0.775	0.225	0.18	1500	-1.15	17.76	-18.2
5	A05	0.875	0.125	0.16	1500	-151	-61	-3.16
6	A06	0.775	0.225	0.18	2500	432.5	11.24	2.479
7	A07	0.775	0.225	0.18	1500	99.93	16.71	-1.11
8	A08	0.825	0.175	0.12	2500	-109	-11.6	13.62
9	A09	0.825	0.175	0.12	2500	-111	10.64	19.92
10	A10	0.875	0.125	0.16	2500	221.6	-50.2	-1.52
11	A11	0.875	0.125	0.16	1500	-226	-37.6	11.74
12	A12	0.825	0.175	0.12	1500	-331	13.58	20.37
13	A13	0.725	0.275	0.14	2500	82.16	59.97	-8.43
14	A14	0.725	0.275	0.14	1500	-290	-17.8	-40.6
15	A15	0.775	0.225	0.18	2500	421.2	15.66	5.832
16	A16	0.825	0.175	0.12	1500	-343	10.7	19.15

Functional DoE Analysis (FDA)

- Functional DOE Analysis
  - Generalized Regression for FPC Scores
    - Generalized Regression for Dissolution FPC 1
    - Generalized Regression for Dissolution FPC 2
    - Generalized Regression for Dissolution FPC 3
  - Diagnostic Plots
  - FDOE Profiler



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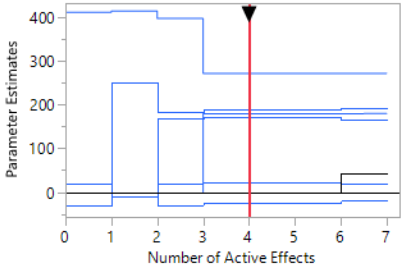
Functional DoE Analysis (FDA)

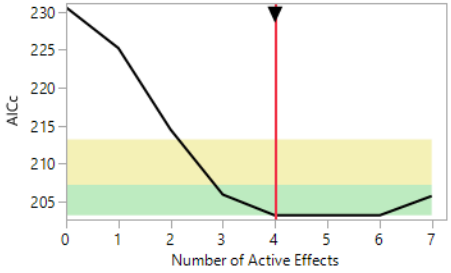
Generalized Regression for FPC Scores

Generalized Regression for Dissolution FPC 1

Normal Best Subset with AICc Validation

Solution Path





Reset Solution

Parameter Estimates for Original Predictors

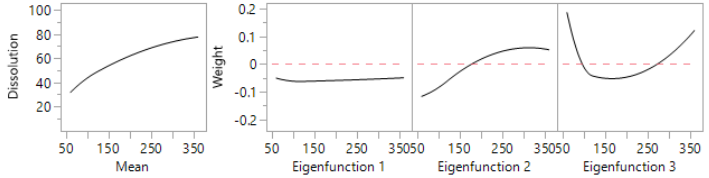
Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	-23.91645	26.485753	0.8153964	0.3665	-75.82757	27.994671
(Polymer B-0.125)/0.15	Forced in	21.35432	15.16401	1.9830943	0.1591	-8.366594	51.075233
Polymer A*Total Polymer		179.73706	52.22562	11.844263	0.0006*	77.376723	282.09739
Polymer A*Compression Force		188.51742	26.823659	49.393171	<.0001*	135.94401	241.09082
Polymer B*Total Polymer		271.97377	36.417342	55.774737	<.0001*	200.59709	343.35044
Polymer B*Compression Force		170.45066	15.599615	119.39045	<.0001*	139.87598	201.02535
Total Polymer*Compression Force		0	0	0	1.0000	0	0

Normal Distribution Parameters	Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale	73.066154	18.560994	15.496372	<.0001*	36.687275	109.44503

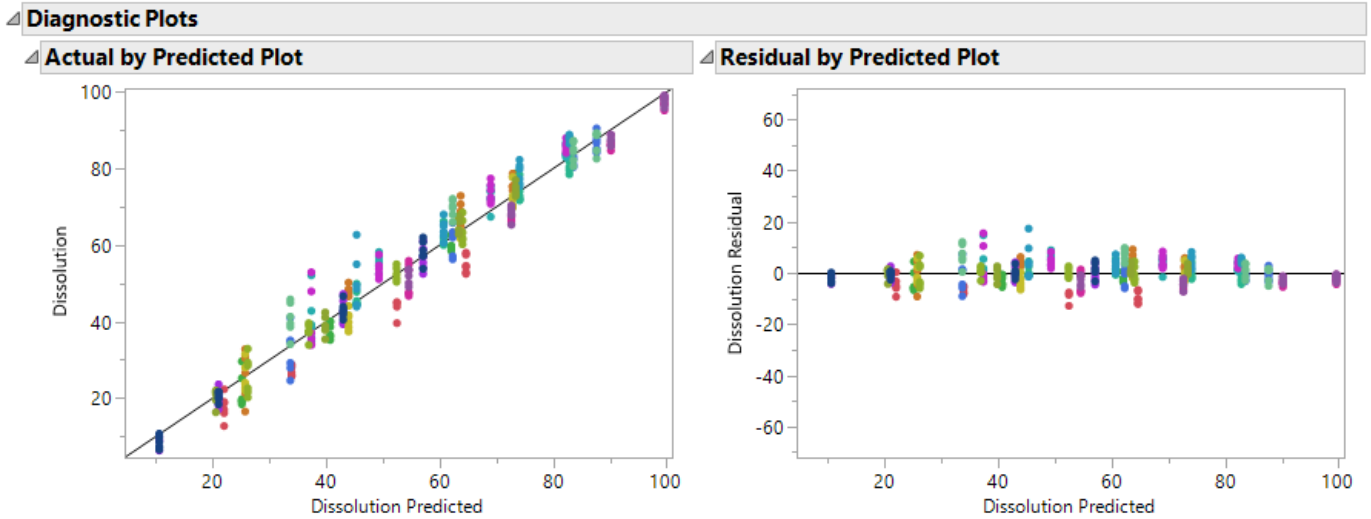
Generalized Regression for Dissolution FPC 2

Generalized Regression for Dissolution FPC 3

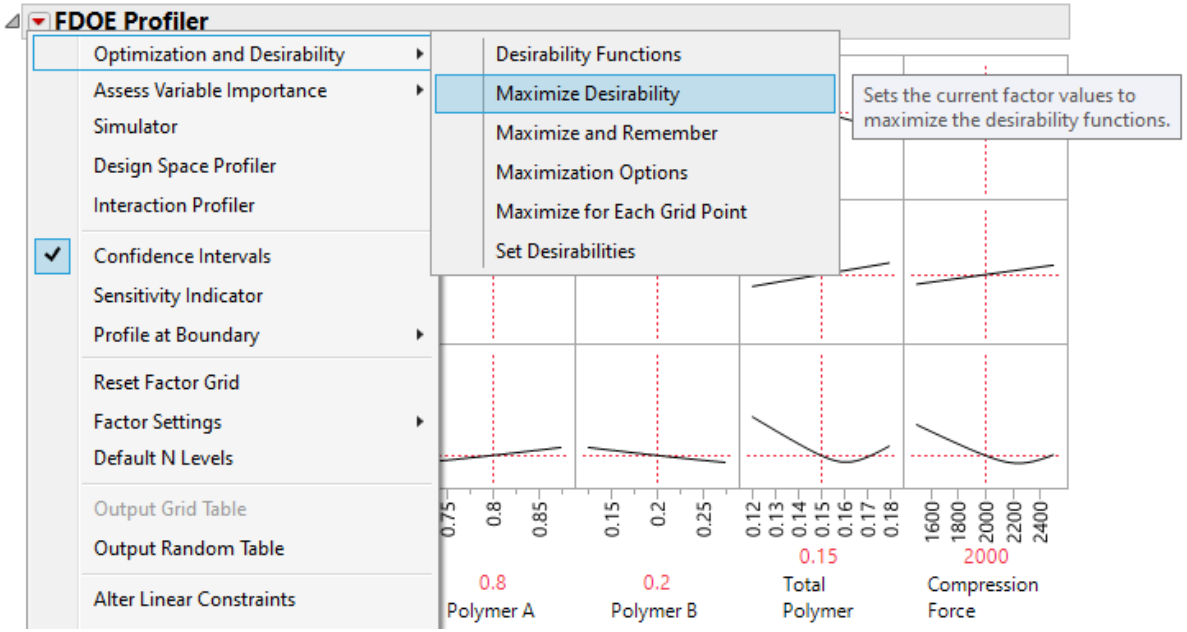
Eigenfunctions



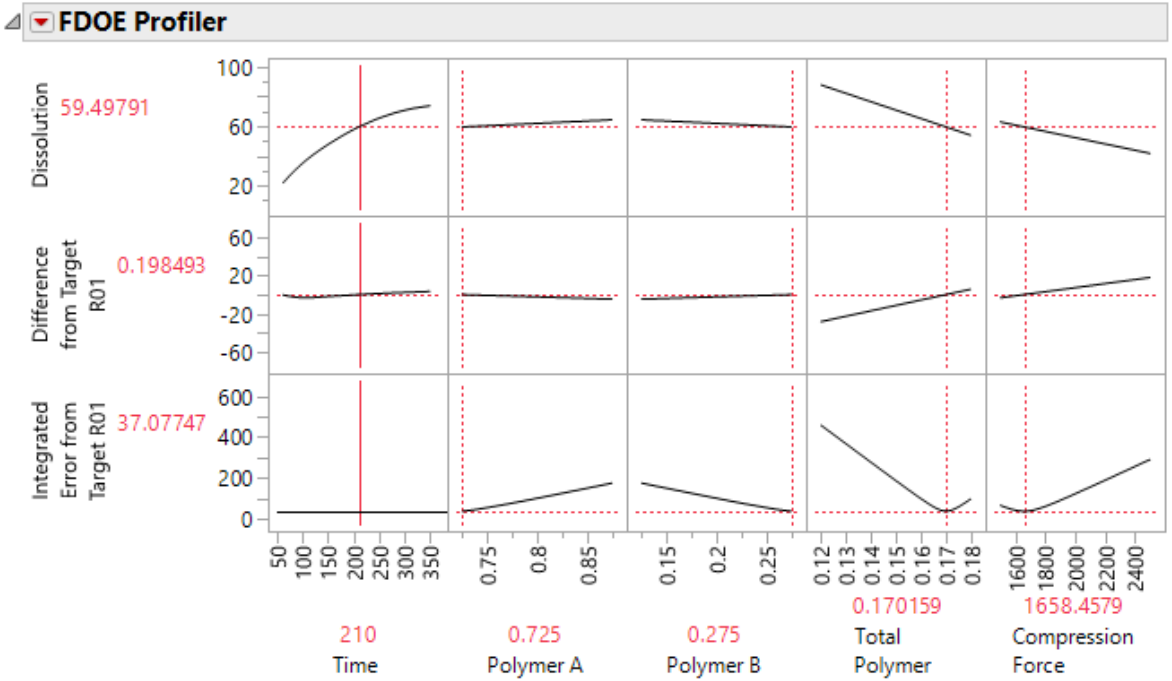
Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)



Functional DoE Analysis (FDA)

Formulation	Polymer A	Polymer B	Total Polymer	Compression Force
f2	0.725	0.275	0.12	2500
FDoE	0.725	0.275	0.17	1700

Curve DoE Analysis (NLR)

1) Fit the reference batch, save prediction formula

2) Curve DoE analysis of the design data, save prediction formula

3) Use Graph<<Profiler to find settings that best match the reference

Curve DoE Analysis (NLR)

Weibull Growth

Prediction Model

$$a \bullet \left(1 - \text{Exp}\left(-\left(\frac{\text{Time}}{b}\right)^{c}\right)\right)$$

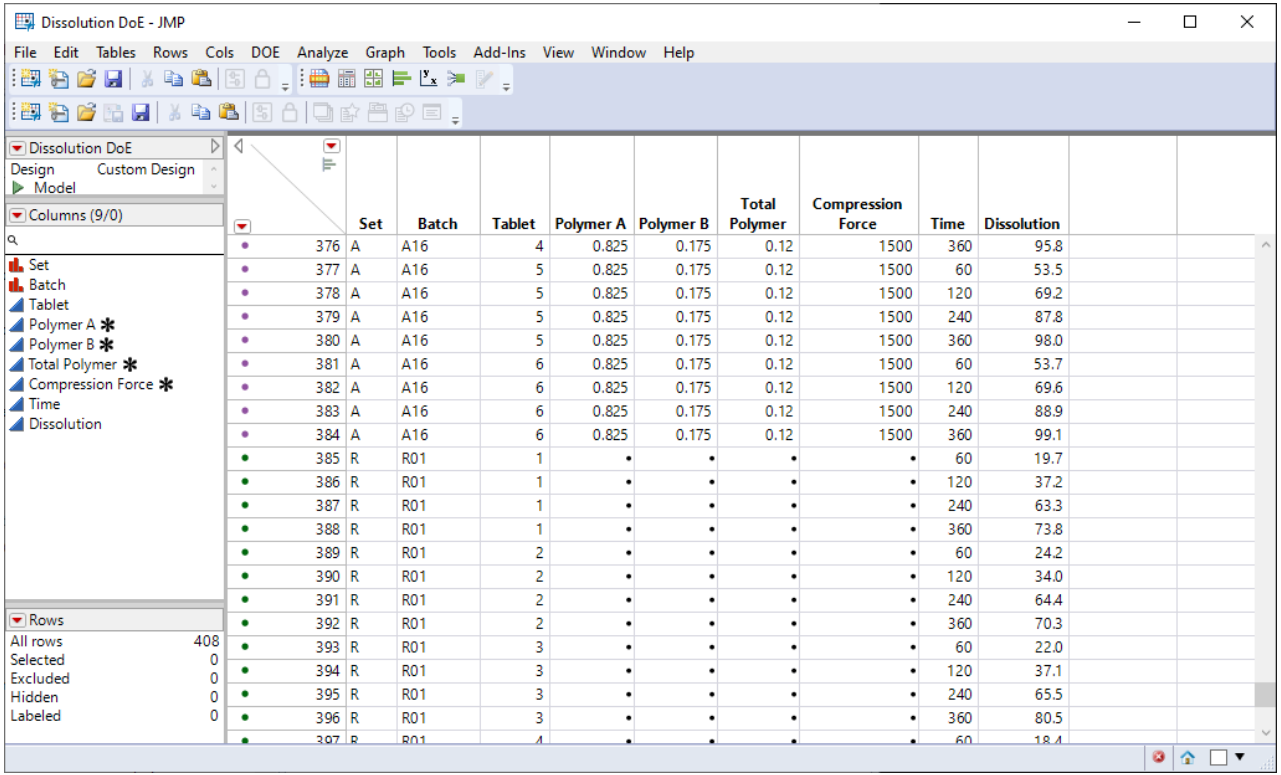
a = Asymptote
b = Inflection Point
c = Growth Rate

Langenbucher, F. Letters to the Editor: Linearization of dissolution rate curves by the Weibull distribution. *J. Pharm. Pharmacol.* 1972, 24 (12), 979–981.

Curve DoE Analysis (NLR)

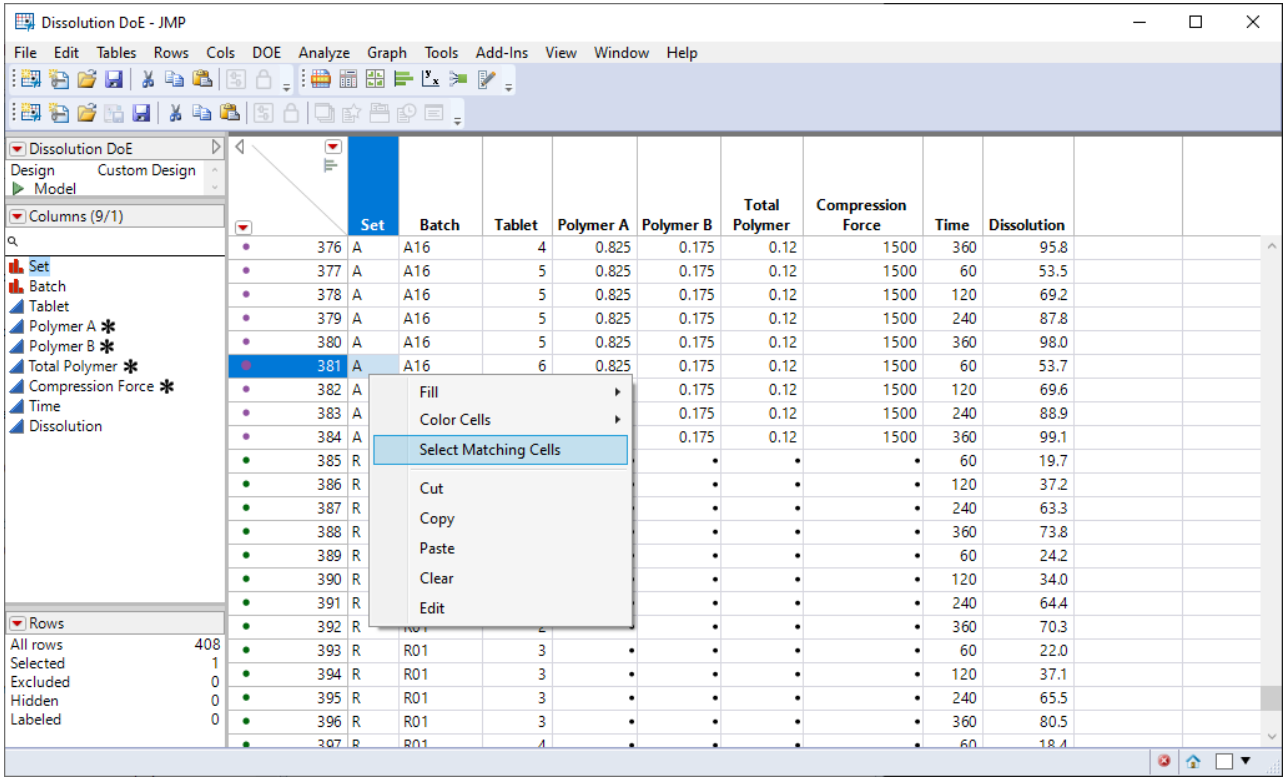
	Batch	Polymer A	Polymer B	Total Polymer	Compression Force	Asymptote	Inflection Point	Growth Rate
1	A01	0.825	0.175	0.16	2500	149.8	1043	0.733
2	A02	0.775	0.225	0.14	2500	104.7	282.5	0.938
3	A03	0.725	0.275	0.14	1500	87.08	107.5	1.311
4	A04	0.775	0.225	0.18	1500	78.78	128.1	1.17
5	A05	0.875	0.125	0.16	1500	91.69	104.5	0.622
6	A06	0.775	0.225	0.18	2500	68.95	248.1	1.454
7	A07	0.775	0.225	0.18	1500	87.61	193.8	0.938
8	A08	0.825	0.175	0.12	2500	150.7	521.5	0.534
9	A09	0.825	0.175	0.12	2500	257.6	2221	0.493
10	A10	0.875	0.125	0.16	2500	199.4	1963	0.565
11	A11	0.875	0.125	0.16	1500	139.6	365.3	0.44
12	A12	0.825	0.175	0.12	1500	135.8	235.2	0.553
13	A13	0.725	0.275	0.14	2500	79.21	158	1.296
14	A14	0.725	0.275	0.14	1500	86.17	83.28	1.356
15	A15	0.775	0.225	0.18	2500	73.12	260.2	1.438
16	A16	0.825	0.175	0.12	1500	131.6	207.9	0.555
17	R01	•	•	•	•	90.65	199.4	1.144

Curve DoE Analysis (NLR)



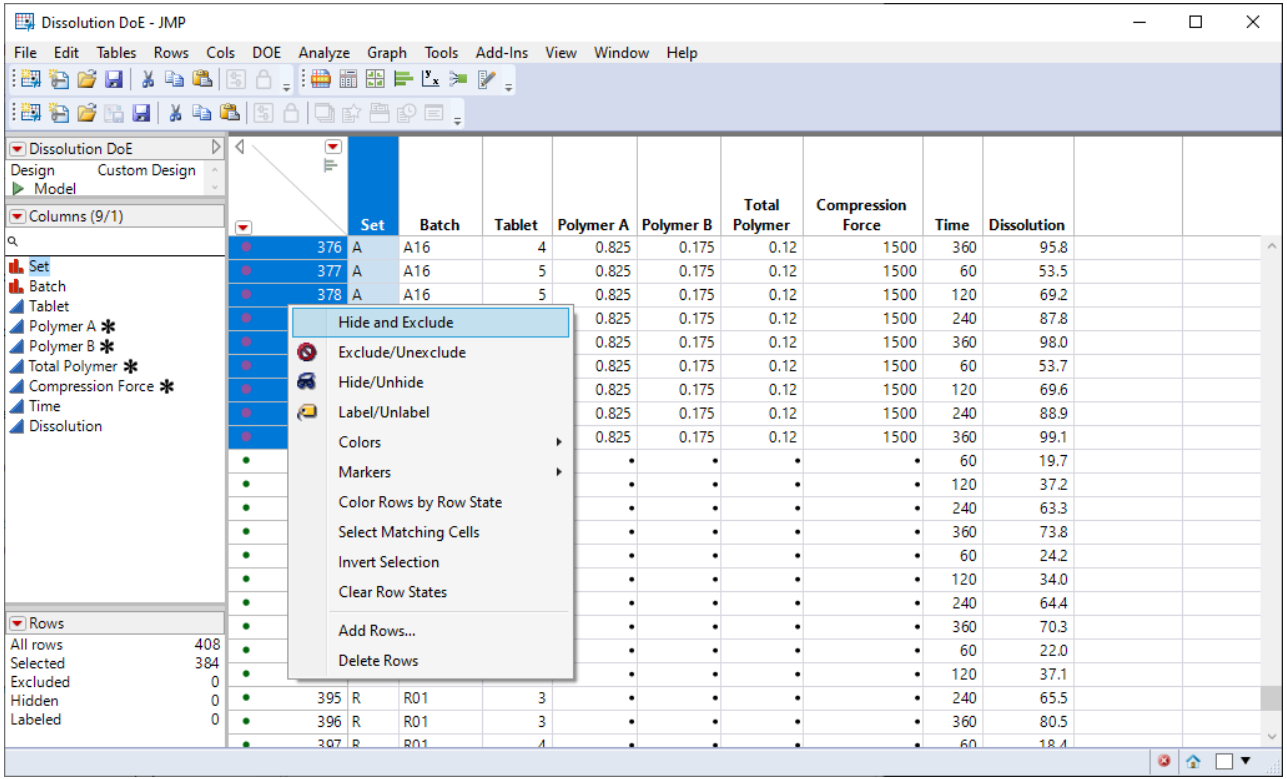
	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
376	A	A16	4	0.825	0.175	0.12	1500	360	95.8
377	A	A16	5	0.825	0.175	0.12	1500	60	53.5
378	A	A16	5	0.825	0.175	0.12	1500	120	69.2
379	A	A16	5	0.825	0.175	0.12	1500	240	87.8
380	A	A16	5	0.825	0.175	0.12	1500	360	98.0
381	A	A16	6	0.825	0.175	0.12	1500	60	53.7
382	A	A16	6	0.825	0.175	0.12	1500	120	69.6
383	A	A16	6	0.825	0.175	0.12	1500	240	88.9
384	A	A16	6	0.825	0.175	0.12	1500	360	99.1
385	R	R01	1	•	•	•	•	60	19.7
386	R	R01	1	•	•	•	•	120	37.2
387	R	R01	1	•	•	•	•	240	63.3
388	R	R01	1	•	•	•	•	360	73.8
389	R	R01	2	•	•	•	•	60	24.2
390	R	R01	2	•	•	•	•	120	34.0
391	R	R01	2	•	•	•	•	240	64.4
392	R	R01	2	•	•	•	•	360	70.3
393	R	R01	3	•	•	•	•	60	22.0
394	R	R01	3	•	•	•	•	120	37.1
395	R	R01	3	•	•	•	•	240	65.5
396	R	R01	3	•	•	•	•	360	80.5

Curve DoE Analysis (NLR)



	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution
376	A	A16	4	0.825	0.175	0.12	1500	360	95.8
377	A	A16	5	0.825	0.175	0.12	1500	60	53.5
378	A	A16	5	0.825	0.175	0.12	1500	120	69.2
379	A	A16	5	0.825	0.175	0.12	1500	240	87.8
380	A	A16	5	0.825	0.175	0.12	1500	360	98.0
381	A	A16	6	0.825	0.175	0.12	1500	60	53.7
382	A				0.175	0.12	1500	120	69.6
383	A				0.175	0.12	1500	240	88.9
384	A				0.175	0.12	1500	360	99.1
385	R				•	•	•	60	19.7
386	R				•	•	•	120	37.2
387	R				•	•	•	240	63.3
388	R				•	•	•	360	73.8
389	R				•	•	•	60	24.2
390	R				•	•	•	120	34.0
391	R				•	•	•	240	64.4
392	R				•	•	•	360	70.3
393	R	R01	3	•	•	•	•	60	22.0
394	R	R01	3	•	•	•	•	120	37.1
395	R	R01	3	•	•	•	•	240	65.5
396	R	R01	3	•	•	•	•	360	80.5

Curve DoE Analysis (NLR)



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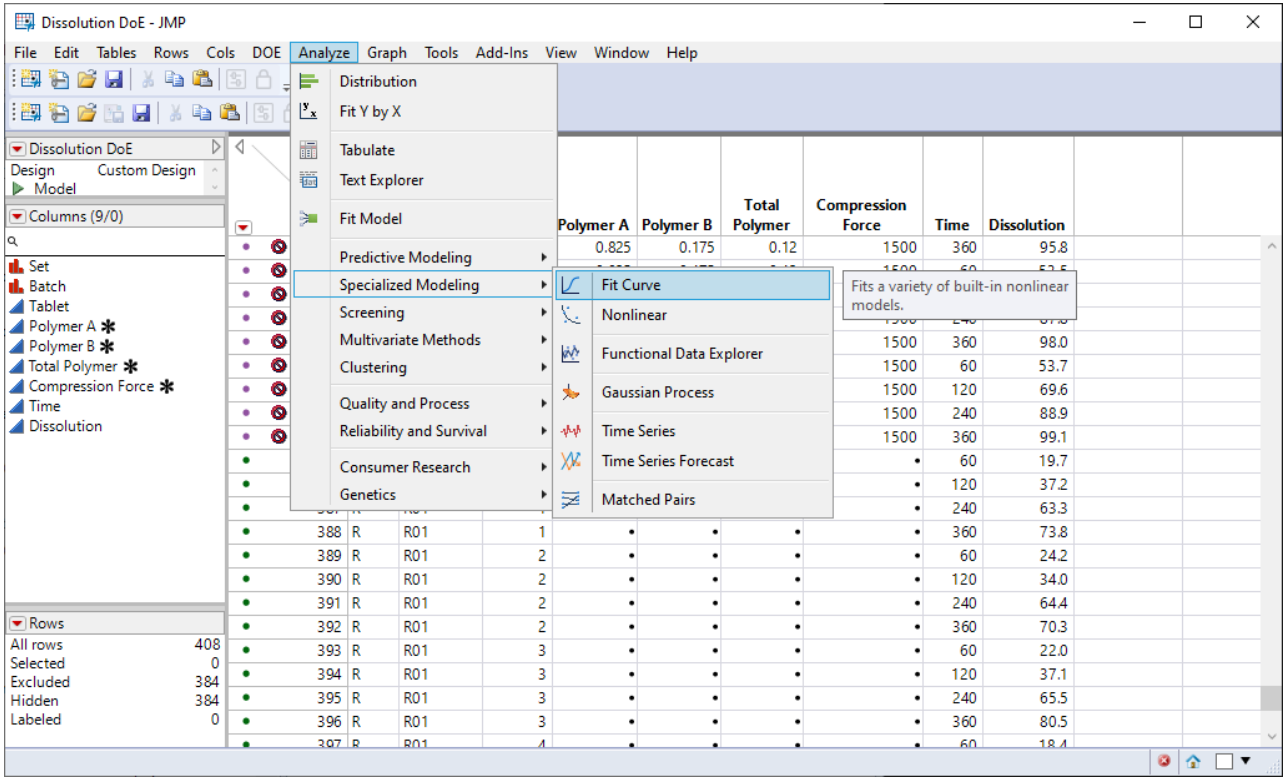

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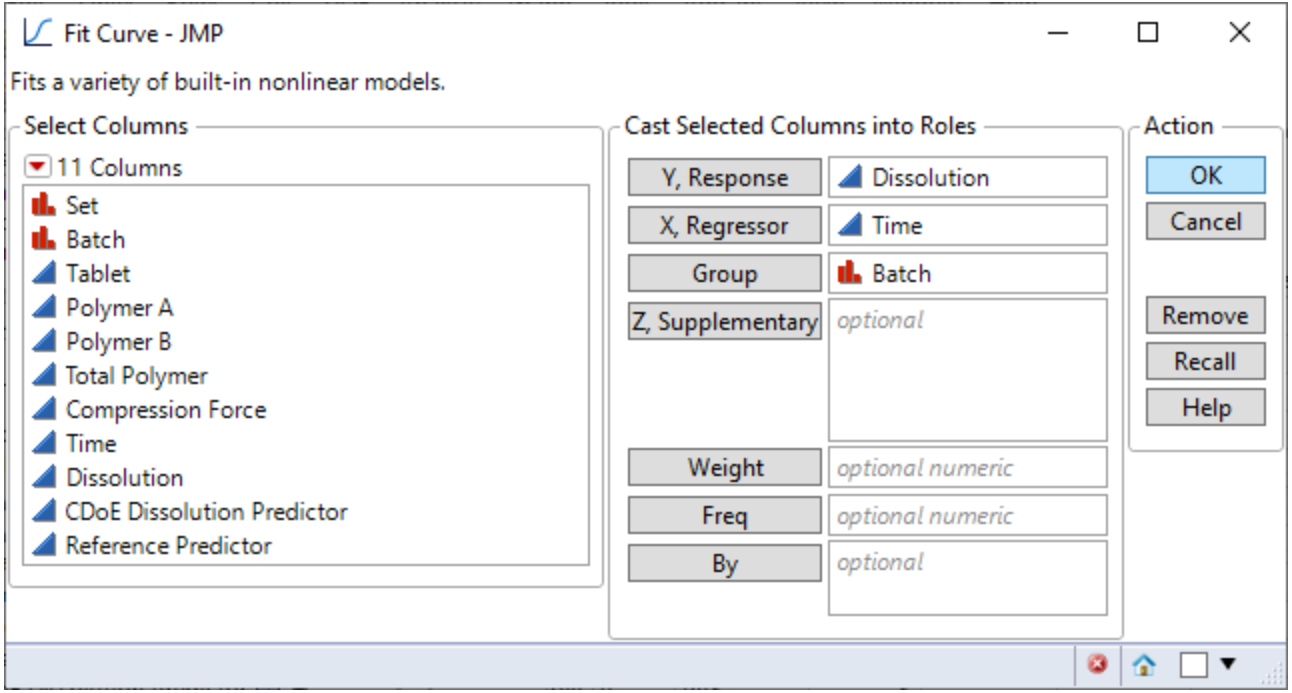

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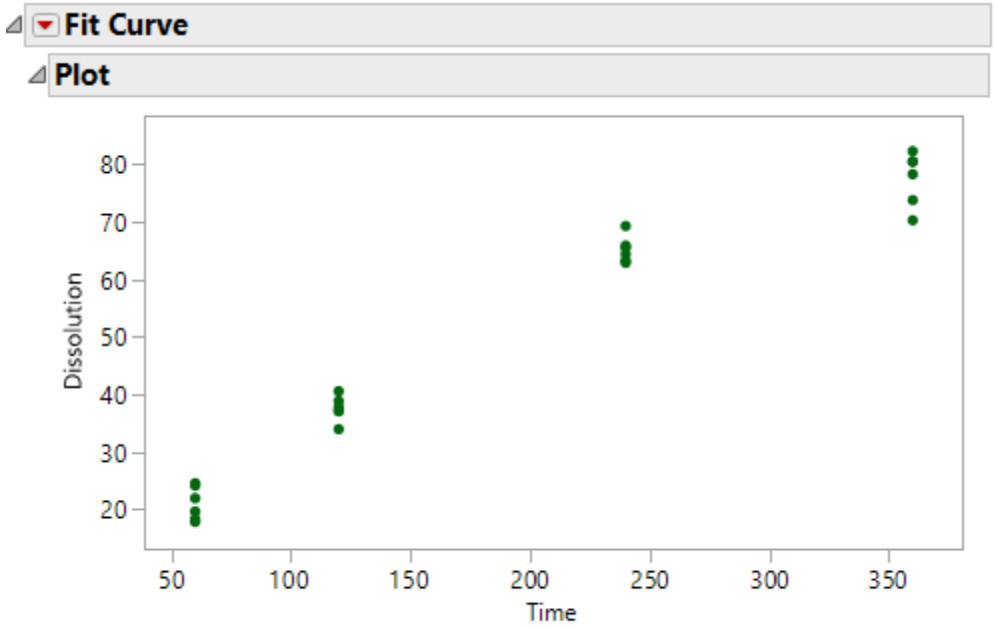

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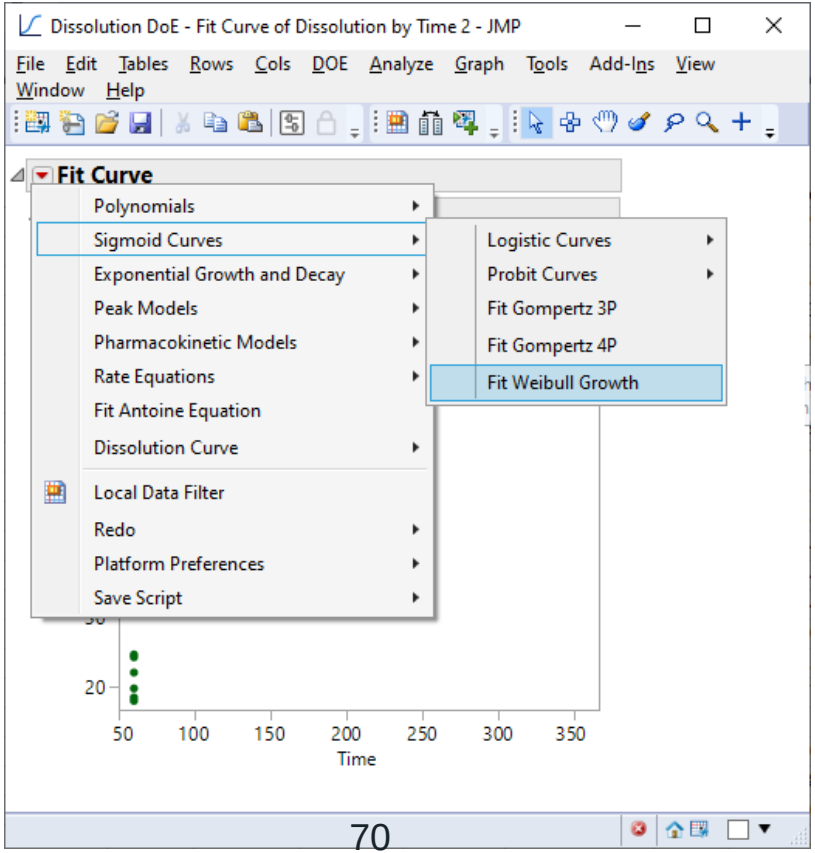
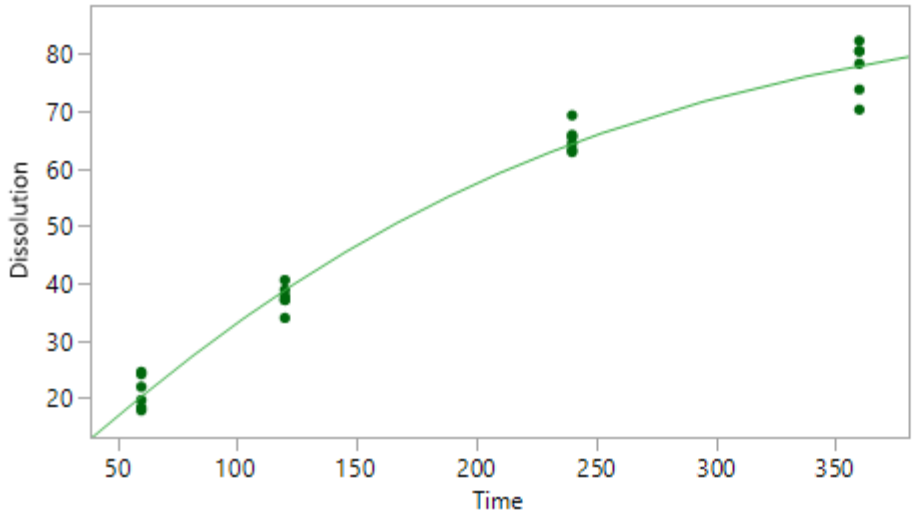


Curve DoE Analysis (NLR)

Fit Curve

Model Comparison

Plot



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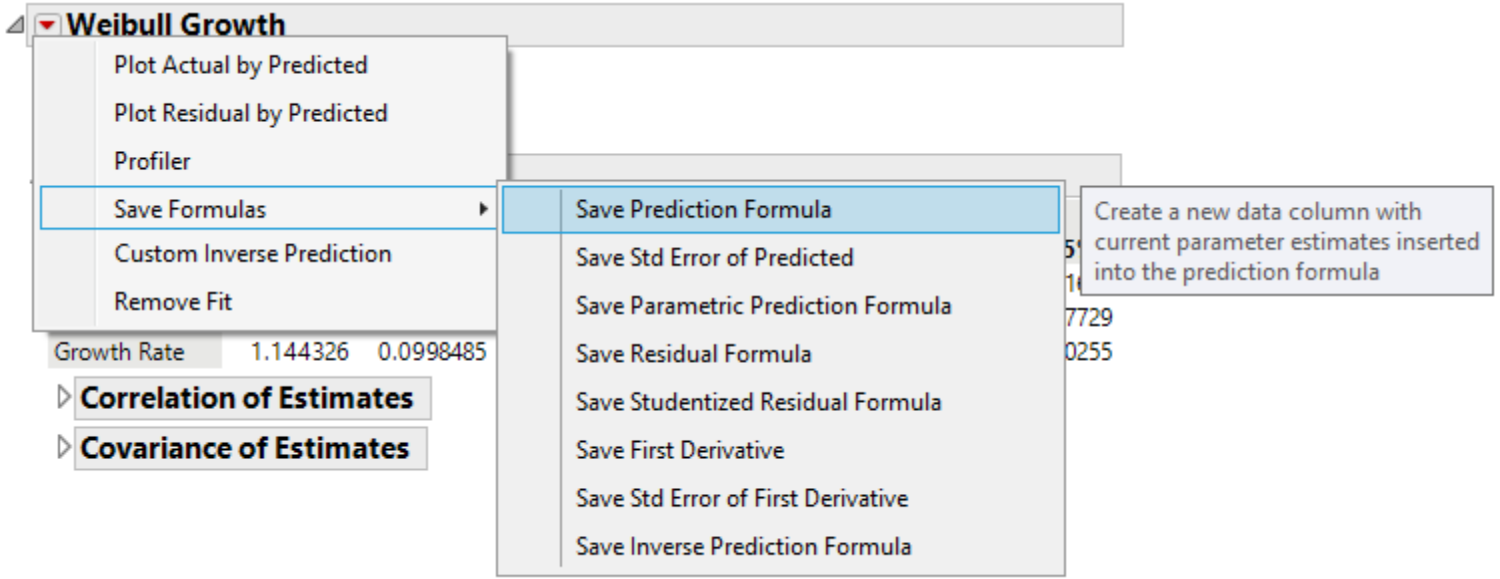


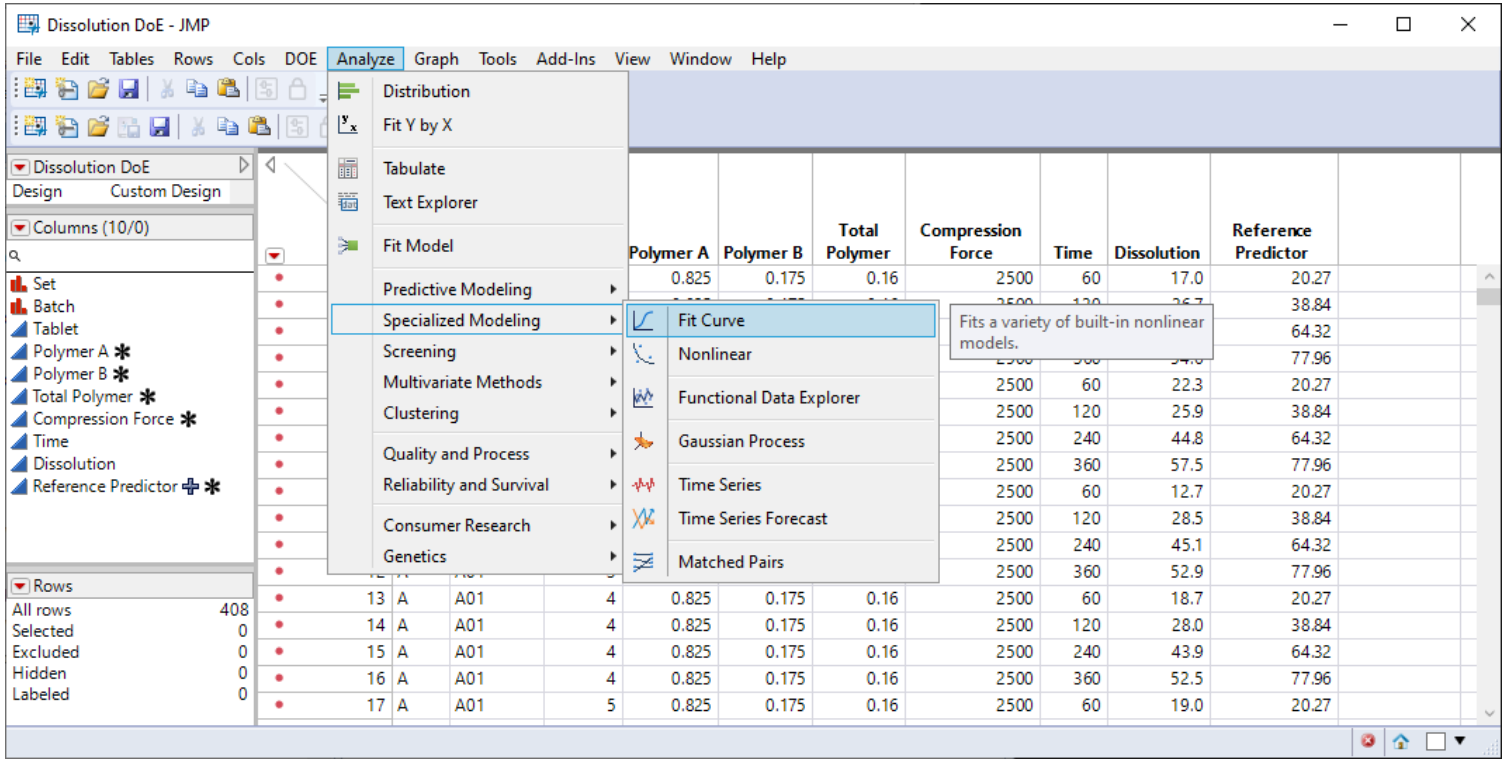
Curve DoE Analysis (NLR)

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	Reference Predictor
1	A	A01	1	0.825	0.175	0.16	2500	60	17.0	20.27
2	A	A01	1	0.825	0.175	0.16	2500	120	26.7	38.84
3	A	A01	1	0.825	0.175	0.16	2500	240	39.6	64.32
4	A	A01	1	0.825	0.175	0.16	2500	360	54.6	77.96
5	A	A01	2	0.825	0.175	0.16	2500	60	22.3	20.27
6	A	A01	2	0.825	0.175	0.16	2500	120	25.9	38.84
7	A	A01	2	0.825	0.175	0.16	2500	240	44.8	64.32
8	A	A01	2	0.825	0.175	0.16	2500	360	57.5	77.96
9	A	A01	3	0.825	0.175	0.16	2500	60	12.7	20.27
10	A	A01	3	0.825	0.175	0.16	2500	120	28.5	38.84
11	A	A01	3	0.825	0.175	0.16	2500	240	45.1	64.32
12	A	A01	3	0.825	0.175	0.16	2500	360	52.9	77.96

Curve DoE Analysis (NLR)

	Set	Batch	Tablet	Polymer A	Polymer B	Total Polymer	Compression Force	Time	Dissolution	Reference Predictor
1	A	A01	1	0.825	0.175	0.16	2500	60	17.0	20.27
2	A	A01	1	0.825	0.175	0.16	2500	120	26.7	38.84
3	A	A01	1	0.825	0.175	0.16	2500	240	39.6	64.32
4	A	A01	1	0.825	0.175	0.16	2500	360	54.6	77.96
5	A	A01	2	0.825	0.175	0.16	2500	60	22.3	20.27
6	A	A01	2	0.825	0.175	0.16	2500	120	25.9	38.84
7	A	A01	2	0.825	0.175	0.16	2500	240	44.8	64.32
8	A	A01	2	0.825	0.175	0.16	2500	360	57.5	77.96
9	A	A01	3	0.825	0.175	0.16	2500	60	12.7	20.27
10	A	A01	3	0.825	0.175	0.16	2500	120	28.5	38.84
11	A	A01	3	0.825	0.175	0.16	2500	240	45.1	64.32
12	A	A01	3	0.825	0.175	0.16	2500	360	52.9	77.96

Curve DoE Analysis (NLR)



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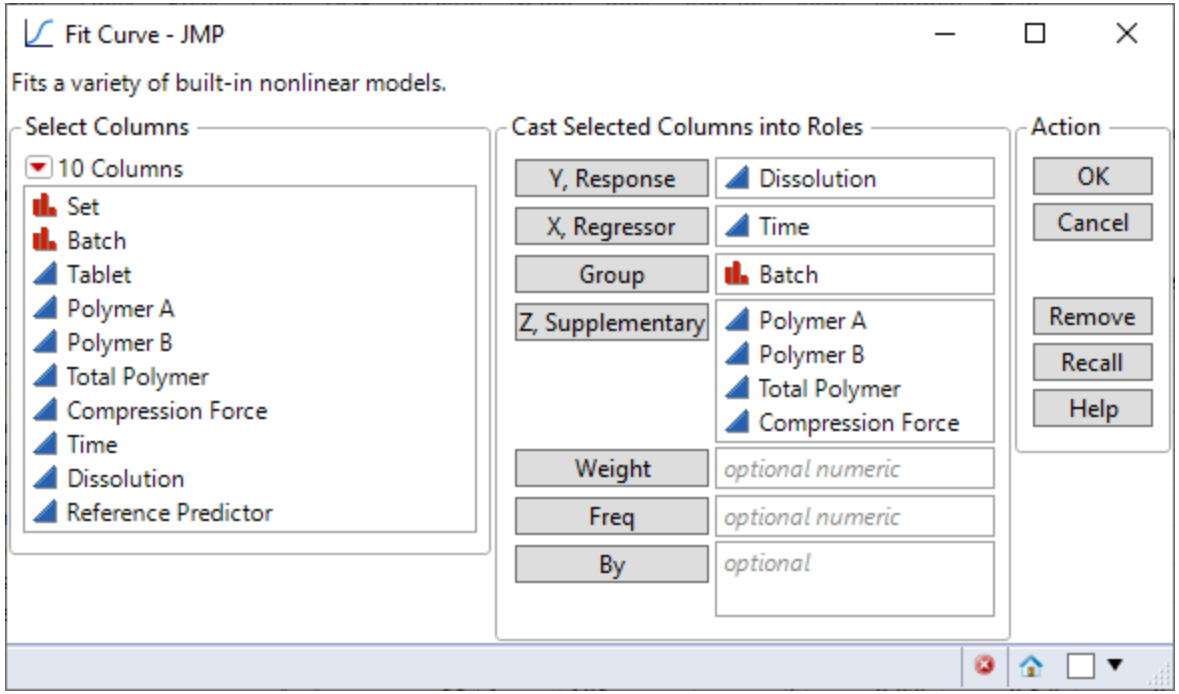

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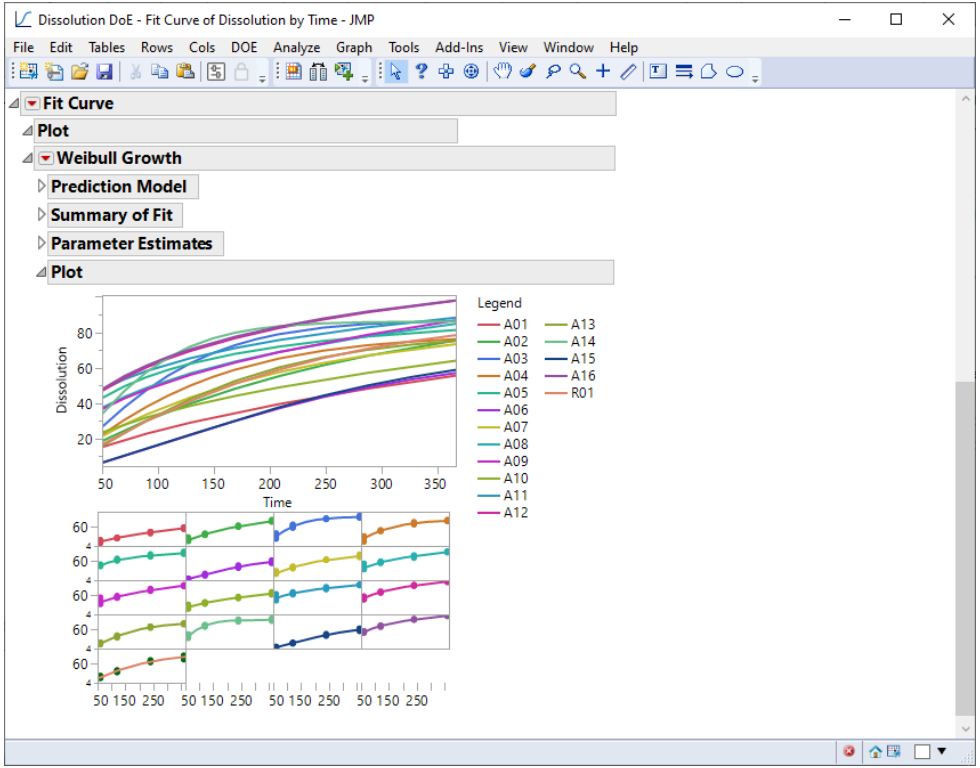
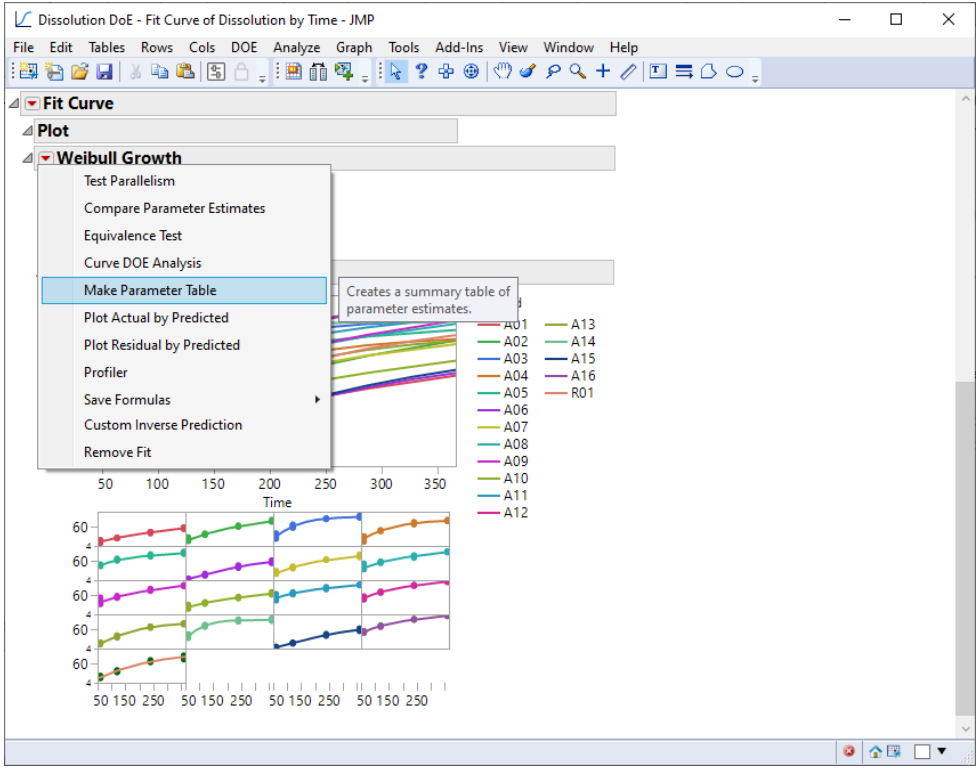


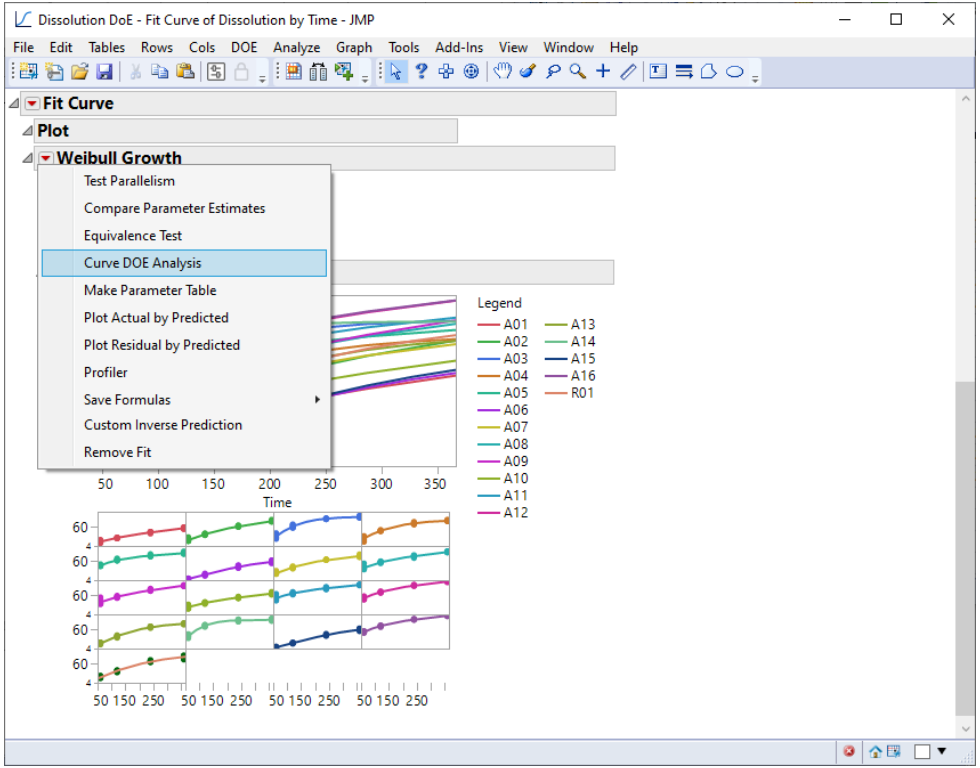
Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)

	Batch	Polymer A	Polymer B	Total Polymer	Compression Force	Asymptote	Inflection Point	Growth Rate
1	A01	0.825	0.175	0.16	2500	149.8	1043	0.733
2	A02	0.775	0.225	0.14	2500	104.7	282.5	0.938
3	A03	0.725	0.275	0.14	1500	87.08	107.5	1.311
4	A04	0.775	0.225	0.18	1500	78.78	128.1	1.17
5	A05	0.875	0.125	0.16	1500	91.69	104.5	0.622
6	A06	0.775	0.225	0.18	2500	68.95	248.1	1.454
7	A07	0.775	0.225	0.18	1500	87.61	193.8	0.938
8	A08	0.825	0.175	0.12	2500	150.7	521.5	0.534
9	A09	0.825	0.175	0.12	2500	257.6	2221	0.493
10	A10	0.875	0.125	0.16	2500	199.4	1963	0.565
11	A11	0.875	0.125	0.16	1500	139.6	365.3	0.44
12	A12	0.825	0.175	0.12	1500	135.8	235.2	0.553
13	A13	0.725	0.275	0.14	2500	79.21	158	1.296
14	A14	0.725	0.275	0.14	1500	86.17	83.28	1.356
15	A15	0.775	0.225	0.18	2500	73.12	260.2	1.438
16	A16	0.825	0.175	0.12	1500	131.6	207.9	0.555
17	R01	•	•	•	•	90.65	199.4	1.144

Curve DoE Analysis (NLR)

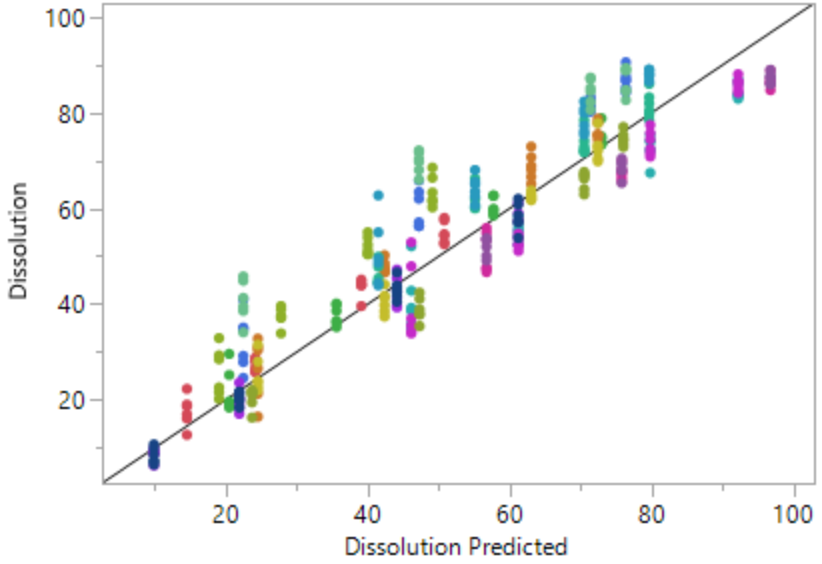


Curve DoE Analysis (NLR)

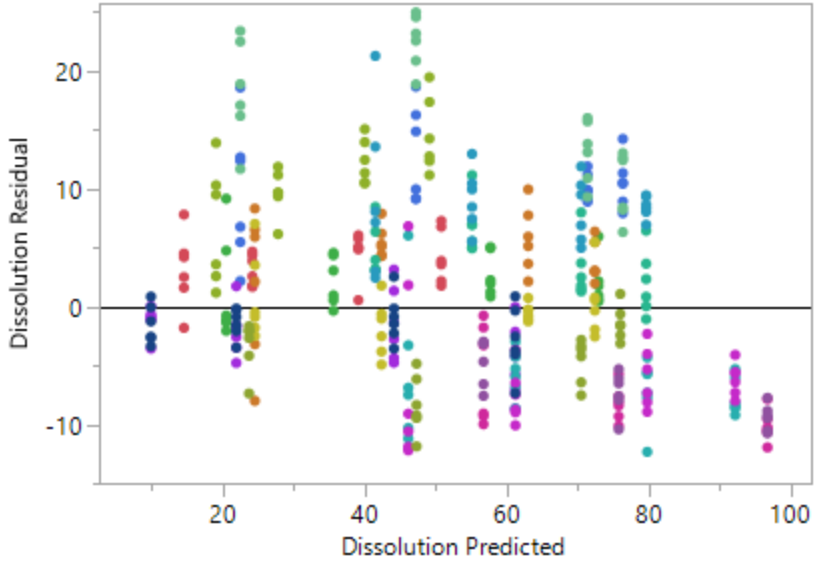
Curve DoE Analysis (NLR)

Diagnostic Plots

Actual by Predicted Plot



Residual by Predicted Plot



Curve DoE Analysis (NLR)

Generalized Regression for Asymptote

LogNormal Best Subset with AICc Validation

Solution Path

Parameter Estimates for Original Predictors

Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	5.0876369	0.0793939	4106.3703	<.0001*	4.9320277	5.2432461
(Polymer B-0.125)/0.15	Forced in	4.3296224	0.0600676	5195.41	<.0001*	4.2118921	4.4473527
Polymer A*Total Polymer		-0.414667	0.1144104	13.136172	0.0003*	-0.638908	-0.190427
Polymer A*Compression Force		0.2397074	0.0718006	11.145676	0.0008*	0.0989808	0.3804341
Polymer B*Total Polymer		0	0	0	1.0000		
Polymer B*Compression Force		0	0	0	1.0000		
Total Polymer*Compression Force		0	0	0	1.0000		

LogNormal Distribution Parameters	Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale	0.1681744	0.0210398	63.890567	<.0001*	0.1269372	0.2094117

$$a \bullet \left(1 - Exp\left(-\left(\frac{Time}{b}\right)^{c}\right)\right)$$

a = Asymptote
b = Inflection Point
c = Growth Rate

Generalized Regression for Inflection Point

Generalized Regression for Growth Rate

Curve DoE Analysis (NLR)

Generalized Regression for Inflection Point

LogNormal Best Subset with AICc Validation

Solution Path

Parameter Estimates for Original Predictors

Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	6.6114613	0.2254624	859.89753	<.0001*	6.1695632	7.0533595
(Polymer B-0.125)/0.15	Forced in	4.7439783	0.1219589	1513.0678	<.0001*	4.5049432	4.9830133
Polymer A*Total Polymer		0	0	0	1.0000	0	0
Polymer A*Compression Force		1.1778766	0.2041102	33.30198	<.0001*	0.7778279	1.5779254
Polymer B*Total Polymer		0	0	0	1.0000		
Polymer B*Compression Force		0	0	0	1.0000		
Total Polymer*Compression Force		0	0	0	1.0000		

LogNormal Distribution Parameters	Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95
Scale	0.3991865	0.0737269	29.315666	<.0001*	0.2546845	0.543688

$$a \bullet \left(1 - \text{Exp}\left(-\left(\frac{\text{Time}}{b}\right)^{c}\right)\right)$$

a = Asymptote
b = Inflection Point
c = Growth Rate

Curve DoE Analysis (NLR)

Generalized Regression for Growth Rate

LogNormal Best Subset with AICc Validation

Solution Path

Parameter Estimates for Original Predictors

Term		Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
(Polymer A-0.725)/0.15	Forced in	-0.716675	0.0561331	163.0071	<.0001*	-0.826694	-0.606656
(Polymer B-0.125)/0.15	Forced in	0.3420244	0.0434337	62.009753	<.0001*	0.2568958	0.4271529
Polymer A*Total Polymer		0.4241638	0.0594451	50.913822	<.0001*	0.3076536	0.5406739
Polymer A*Compression Force		0	0	0	1.0000	0	0
Polymer B*Total Polymer		0	0	0	1.0000		
Polymer B*Compression Force		0	0	0	1.0000		
Total Polymer*Compression Force		0.0928903	0.0337311	7.5836617	0.0059*		

LogNormal Distribution Parameters	Estimate	Std Error	Wald ChiSquare	Prob > ChiSquare	Lower 95%	Upper 95%
Scale	0.1035127	0.0140294	54.439018	<.0001*	0.0760156	0.1310098

$$a \bullet \left(1 - \text{Exp}\left(-\left(\frac{\text{Time}}{b}\right)^{c}\right)\right)$$

a = Asymptote
b = Inflection Point
c = Growth Rate

Curve DoE Analysis (NLR)

```
Exp(
    5.08763690244406 * ((:Polymer A - 0.725) / 0.15) + 4.32962237609893 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Total Polymer - 0.15) / 0.03) * -0.414667337719225) + ((:Polymer A - 0.725) / 0.15) * (((:Compression Force - 2000) / 500) * 0.239707444419611)
     + 0.168174449903471 ^ 2 / 2
) * (1 - Exp(
    -(:Time / Exp(
        6.61146132683894 * ((:Polymer A - 0.725) / 0.15) + 4.74397829394421 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
        :Compression Force - 2000) / 500) * 1.17787664936899) + 0.399186546036449 ^ 2 / 2
    )) ^ Exp(
        -0.716674955680227 * ((:Polymer A - 0.725) / 0.15) + 0.342024361999155 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
        :Total Polymer - 0.15) / 0.03) * 0.424163753840414) + ((:Total Polymer - 0.15) / 0.03) * (((:Compression Force - 2000) / 500) *
        0.0928902831533859) + 0.103512708322975 ^ 2 / 2
    )
))
```

$$a \cdot \left(1 - \mathrm{Exp}\left(-\left(\frac{\mathrm{Time}}{b}\right)^{c}\right)\right)$$

a = Asymptote
b = Inflection Point
c = Growth Rate

Curve DoE Analysis (NLR)

```
Exp(
    5.08763690244406 * ((:Polymer A - 0.725) / 0.15) + 4.32962237609893 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
    :Total Polymer - 0.15) / 0.03) * -0.414667337719225) + ((:Polymer A - 0.725) / 0.15) * (((:Compression Force - 2000) / 500) * 0.239707444419611)
     + 0.168174449903471 ^ 2 / 2
) * (1 - Exp(
    -(:Time / Exp(
        6.61146132683894 * ((:Polymer A - 0.725) / 0.15) + 4.74397829394421 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
        :Compression Force - 2000) / 500) * 1.17787664936899) + 0.399186546036449 ^ 2 / 2
    )) ^ Exp(
        -0.716674955680227 * ((:Polymer A - 0.725) / 0.15) + 0.342024361999155 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
        :Total Polymer - 0.15) / 0.03) * 0.424163753840414) + ((:Total Polymer - 0.15) / 0.03) * (((:Compression Force - 2000) / 500) *
        0.0928902831533859) + 0.103512708322975 ^ 2 / 2
    )
))
```

$$a \cdot \left(1 - \mathrm{Exp}\left(-\left(\frac{\mathrm{Time}}{b}\right)^{c}\right)\right)$$

a = Asymptote
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Curve DoE Analysis (NLR)

```
Exp(
    5.08763690244406 * ((:Polymer A - 0.725) / 0.15) + 4.32962237609893 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
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     + 0.168174449903471 ^ 2 / 2
) * (1 - Exp(
    -(:Time / Exp(
        6.61146132683894 * ((:Polymer A - 0.725) / 0.15) + 4.74397829394421 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
        :Compression Force - 2000) / 500) * 1.17787664936899) + 0.399186546036449 ^ 2 / 2
    )) ^ Exp(
        -0.716674955680227 * ((:Polymer A - 0.725) / 0.15) + 0.342024361999155 * ((:Polymer B - 0.125) / 0.15) + ((:Polymer A - 0.725) / 0.15) * (((
        :Total Polymer - 0.15) / 0.03) * 0.424163753840414) + ((:Total Polymer - 0.15) / 0.03) * (((:Compression Force - 2000) / 500) *
        0.0928902831533859) + 0.103512708322975 ^ 2 / 2
    )
))
```

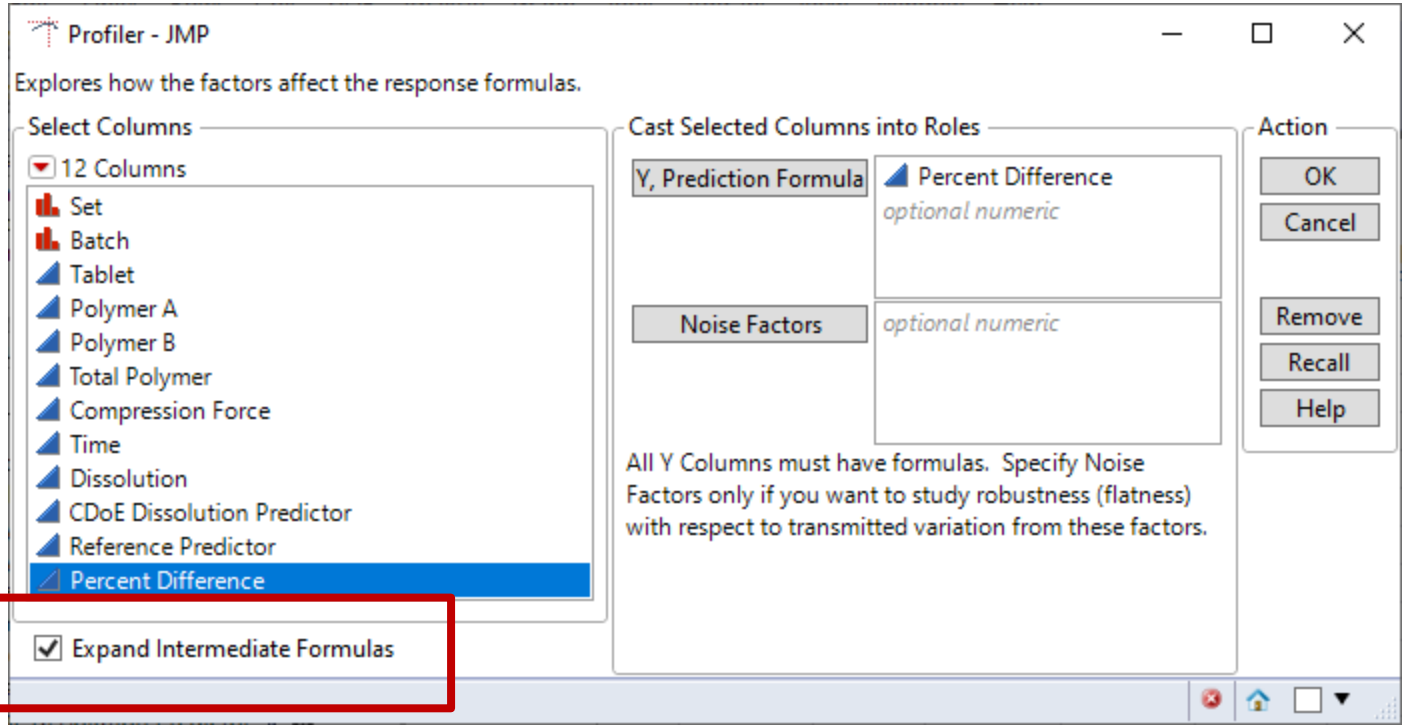
$$a \cdot \left(1 - \mathrm{Exp}\left(-\left(\frac{\mathrm{Time}}{b}\right)^{c}\right)\right)$$

a = Asymptote
b = Inflection Point
c = Growth Rate

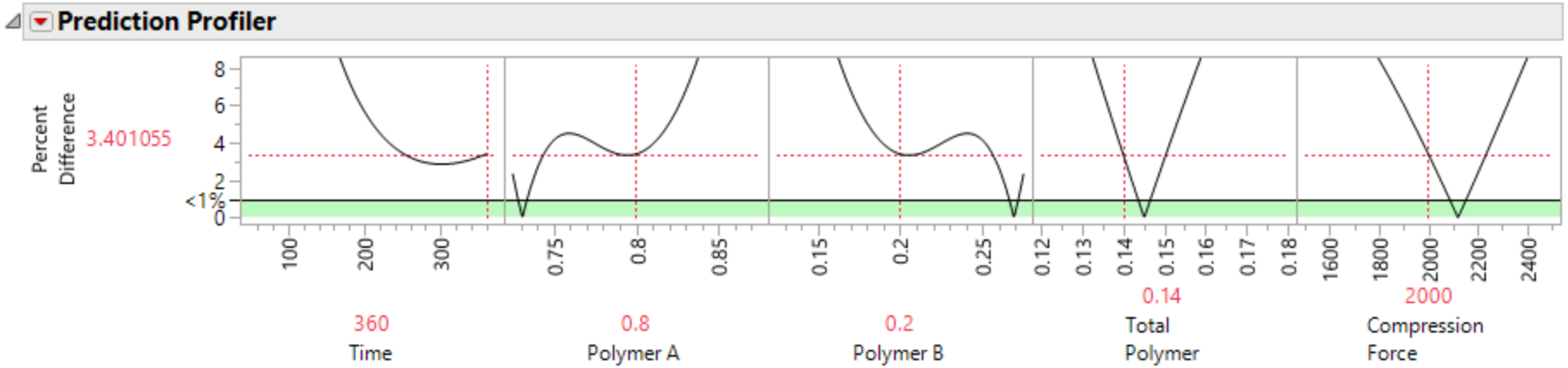
Curve DoE Analysis (NLR)

$$100 \cdot \left(\frac{\left| \text{CDoE Dissolution Predictor} - \text{Reference Predictor} \right|}{\text{Reference Predictor}} \right)$$

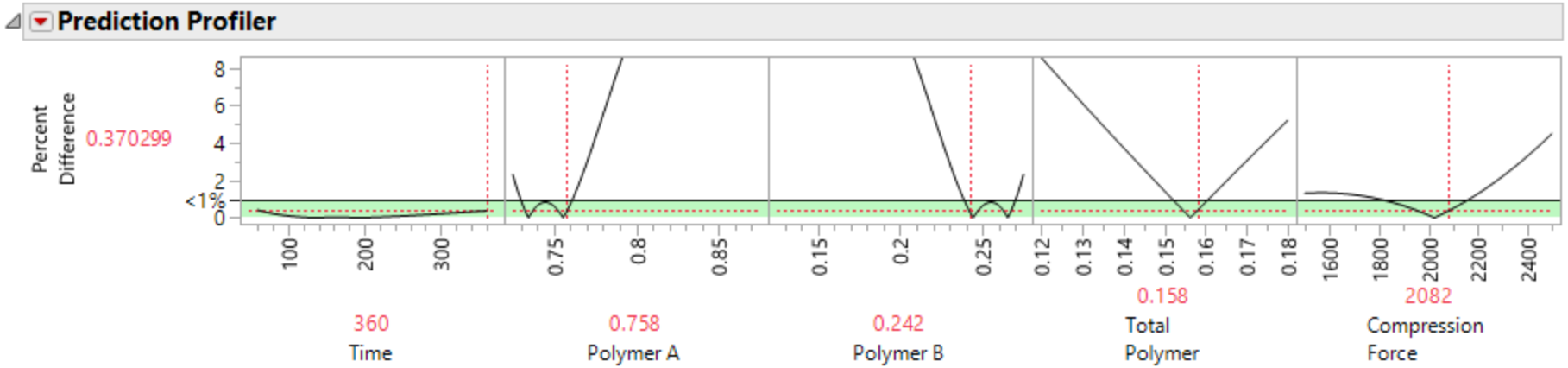
Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)



Curve DoE Analysis (NLR)



Verification Results

f2

FDA

NLR

	Formulation	Polymer A	Polymer B	Total Polymer	Compression Force
1	Ref	•	•	•	•
2	f2	0.725	0.275	0.12	2500
3	FDoE	0.725	0.275	0.17	1700
4	CDoE	0.758	0.242	0.16	2100

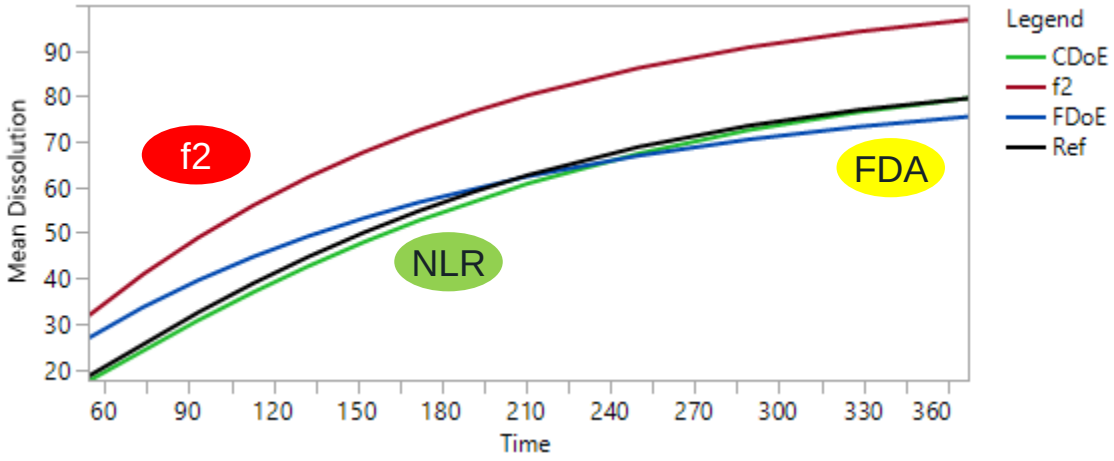
Verification Results

	Formulation	Rep	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60	Dissolution 120	Dissolution 240	Dissolution 360
1	Ref	1	•	•	•	•	22.9	41.1	71.9	82.1
2	Ref	2	•	•	•	•	17.7	40.7	66.8	77
3	Ref	3	•	•	•	•	22.7	42.9	68.7	79.1
4	Ref	4	•	•	•	•	21.8	39.8	68.5	79.6
5	Ref	5	•	•	•	•	19.3	39.7	65.8	79.2
6	Ref	6	•	•	•	•	20.9	40.1	64.7	77.1
7	CDoE	1	0.758	0.242	0.16	2100	17.8	43	67.2	80.2
8	CDoE	2	0.758	0.242	0.16	2100	23.4	38.8	66.7	78.3
9	CDoE	3	0.758	0.242	0.16	2100	20.3	36.3	63.1	77.3
10	CDoE	4	0.758	0.242	0.16	2100	18.9	42.2	66.6	79
11	CDoE	5	0.758	0.242	0.16	2100	18.9	39.3	67	81.1
12	CDoE	6	0.758	0.242	0.16	2100	15.6	37.2	63.1	79.2
13	FDoE	1	0.725	0.275	0.17	1700	31.6	52.1	62.8	75.5
14	FDoE	2	0.725	0.275	0.17	1700	28.8	49.2	60.5	76
15	FDoE	3	0.725	0.275	0.17	1700	23.3	48.4	64.3	75.7
16	FDoE	4	0.725	0.275	0.17	1700	29.2	50.3	64.4	76.8
17	FDoE	5	0.725	0.275	0.17	1700	24.9	46.7	61.7	74.1
18	FDoE	6	0.725	0.275	0.17	1700	24.9	52.3	63.3	80.8
19	f2	1	0.725	0.275	0.12	2500	31.3	57.8	86.4	96
20	f2	2	0.725	0.275	0.12	2500	25.6	54.2	79.7	94.7
21	f2	3	0.725	0.275	0.12	2500	36.1	57.6	83.6	95.7
22	f2	4	0.725	0.275	0.12	2500	38.3	59.4	84.5	96.8
23	f2	5	0.725	0.275	0.12	2500	32.2	61.9	91.8	98.2
24	f2	6	0.725	0.275	0.12	2500	45.3	57.3	85.1	96.1
25	BCV	1	0.725	0.275	0.17	1750	17	46.9	69.1	84.1
26	BCV	2	0.725	0.275	0.17	1750	23.6	45.6	72.7	88.9
27	BCV	3	0.725	0.275	0.17	1750	20.4	41.8	75.5	87.5
28	BCV	4	0.725	0.275	0.17	1750	16.9	47.6	72.9	82.9
29	BCV	5	0.725	0.275	0.17	1750	25.4	46	65.2	83.9
30	BCV	6	0.725	0.275	0.17	1750	21	47	67.8	77.5

Verification Results

		Formulation	Polymer A	Polymer B	Total Polymer	Compression Force	Dissolution 60 Mean	Dissolution 120 Mean	Dissolution 240 Mean	Dissolution 360 Mean	f2
	1	Ref	•	•	•	•	20.88	40.72	67.73	79.02	100
f2	2	f2	0.725	0.275	0.12	2500	34.80	58.03	85.18	96.25	39.03
FDA	3	FDoE	0.725	0.275	0.17	1700	27.12	49.83	62.83	76.48	60.2
NLR	4	CDoE	0.758	0.242	0.16	2100	19.15	39.47	65.62	79.18	87.16

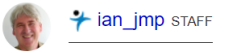
Verification Results



InfoQ Assessment of Results

	f2	FDoE	CDoE
Generalizability	Insufficient	Good	Best
Operationalization	Good/Easy	Good/Easy	Good/Harder
Communication	Good	Good	Best

f2 FDA NLR

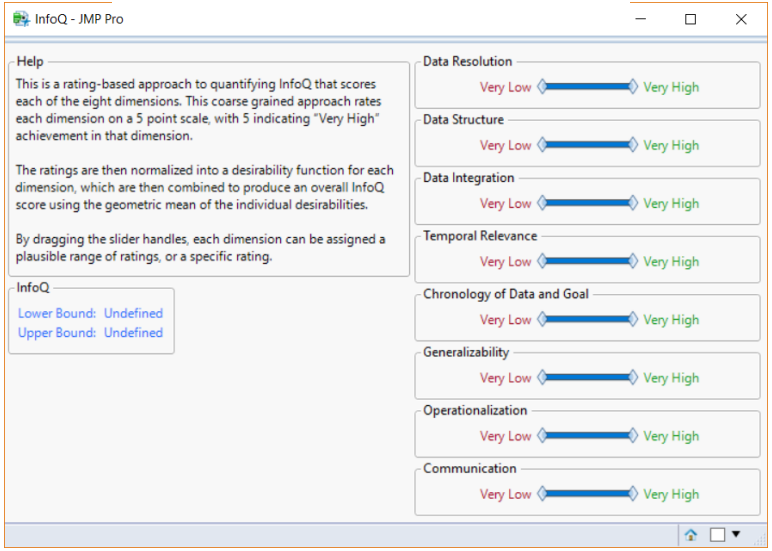


ian_jmp STAFF

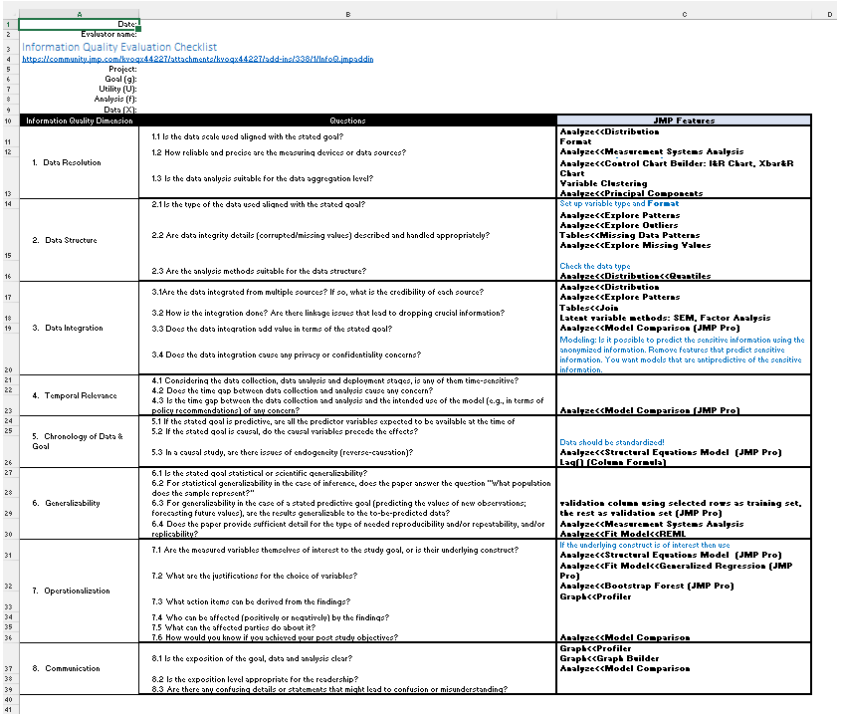
Calculate 'InfoQ' score with JMP

Created: **JAN 24, 2017 09:26 AM** | Last Modified: **JAN 24, 2017 12:15 PM**

InfoQ.jmpaddin



https://community.jmp.com/t5/JMP-Add-Ins/Calculate-InfoQ-score-with-JMP/ta-p/34898



Date:
Evaluator name:

Information Quality Evaluation Checklist

https://community.jmp.com/kvoqx44227/attachments/kvoqx44227/add-ins/338/1/InfoQ.jmpaddin

Project:
Goal (g):
Utility (U):
Analysis (f):
Data (X):

Information Quality Dimension	Questions	JMP Features
1. Data Resolution	1.1 Is the data scale used aligned with the stated goal? 1.2 How reliable and precise are the measuring devices or data sources? 1.3 Is the data analysis suitable for the data aggregation level?	Analyze<<Distribution Format Analyze<<Measurement Systems Analysis Analyze<<Control Chart Builder: I&R Chart, Xbar&R Chart Variable Clustering Analyze<<Principal Components
2. Data Structure	2.1 Is the type of the data used aligned with the stated goal? 2.2 Are data integrity details (corrupted/missing values) described and handled appropriately? 2.3 Are the analysis methods suitable for the data structure?	Set up variable type and Format Analyze<<Explore Patterns Analyze<<Explore Outliers Tables<<Missing Data Patterns Analyze<<Explore Missing Values Check the data type Analyze<<Distribution<<Quantiles
3. Data Integration	3.1Are the data integrated from multiple sources? If so, what is the credibility of each source? 3.2 How is the integration done? Are there linkage issues that lead to dropping crucial information? 3.3 Does the data integration add value in terms of the stated goal? 3.4 Does the data integration cause any privacy or confidentiality concerns?	Analyze<<Distribution Analyze<<Explore Patterns Tables<<Join Latest variable methods: SEM, Factor Analysis Analyze<<Model Comparison (JMP Pro) Modeling: Is it possible to predict the sensitive information using the anonymized information. Remove features that predict sensitive information. You want models that are unpredictive of the sensitive information.
4. Temporal Relevance	4.1 Considering the data collection, data analysis and deployment stages, is any of them time-sensitive? 4.2 Does the time gap between data collection and analysis cause any concern? 4.3 Is the time gap between the data collection and analysis and the intended use of the model (e.g., in terms of policy recommendations) of any concern?	Analyze<<Model Comparison (JMP Pro)
5. Chronology of Data & Goal	5.1 If the stated goal is predictive, are all the predictor variables expected to be available at the time of 5.2 If the stated goal is causal, do the causal variables precede the effects? 5.3 In a causal study, are there issues of endogeneity (reverse-causation)?	Data should be standardized! Analyze<<Structural Equations Model (JMP Pro) Lag() (Column Formula)
6. Generalizability	6.1 Is the stated goal statistical or scientific generalizability? 6.2 For statistical generalizability in the case of inference, does the paper answer the question "What population does the sample represent?" 6.3 For generalizability in the case of a stated predictive goal (predicting the values of new observations; forecasting future values), are the results generalizable to the to-be-predicted data? 6.4 Does the paper provide sufficient detail for the type of needed reproducibility and/or repeatability, and/or replicability?	validation column using selected rows as training set, the rest as validation set (JMP Pro) Analyze<<Measurement Systems Analysis Analyze<<Fit Model<<REML
7. Operationalization	7.1 Are the measured variables themselves of interest to the study goal, or is their underlying construct? 7.2 What are the justifications for the choice of variables? 7.3 What action items can be derived from the findings? 7.4 Who can be affected (positively or negatively) by the findings? 7.5 What can the affected parties do about it? 7.6 How would you know if you achieved your post study objectives?	If the underlying construct is of interest then use Analyze<<Structural Equations Model (JMP Pro) Analyze<<Fit Model<<Generalized Regression (JMP Pro) Analyze<<Bootstrap Forest (JMP Pro) Graph<<Profiler Analyze<<Model Comparison
8. Communication	8.1 Is the exposition of the goal, data and analysis clear? 8.2 Is the exposition level appropriate for the readership? 8.3 Are there any confusing details or statements that might lead to confusion or misunderstanding?	Graph<<Profiler Graph<<Graph Builder Analyze<<Model Comparison

https://community.jmp.com/t5/Discovery-Summit-Europe-2021/Maximizing-Data-Science-Success-with-Information-Quality-InfoQ/ta-p/349217?attachment-id=12709

Thank you for your attention

KPA Insights through analytics

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