Optimization of arsenic extraction in rice samples by Plackett-Burman design and response surface methodology

The objective of this research paper is to optimize the extraction condition of arsenic species and dimethylarsonic acid in paddy rice by a simple solvent extraction using water as an extraction reagent. Design of experiments (DoE) methodology is implemented for the estimation of the variable effects.

The factors (independent variables) examined are: T = extraction temperature (°C), t = shaking time (min), R = rotation speed (rpm), V = solvent volume (mL) and D = dummy factor. All the factors are continuous. The responses (dependent variables) examined are: Y_1 = As (III) extraction (mg/kg), Y_2 = As (V) (mg/kg), Y_3 = DMA extraction (mg/kg) and Y_4 = sum of arsenic species (mg/kg). The applied DoE method is Plackett Burman design.

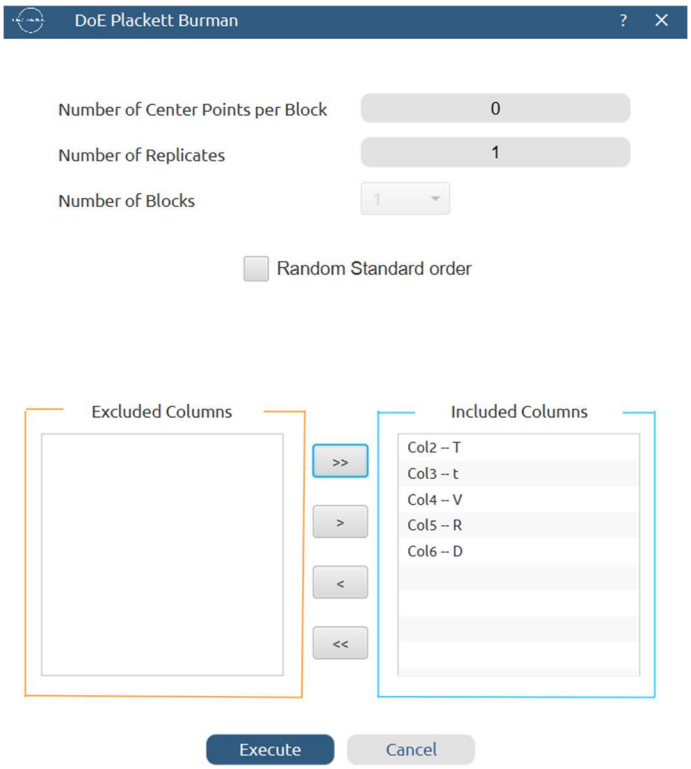
Isalos version used: 2.0.6

Scientific article: https://www.sciencedirect.com/science/article/abs/pii/S0308814616302977

Step 1: Plackett Burman Design

In the first tab named “Action” define the factors in the column headers and fill each column with the low and high levels of the corresponding factors. This tab can be renamed “Plackett Burman”. Afterwards, apply the Plackett Burman method: *DOE → Screening → Plackett Burman*

	Col1	Col2 (I)	Col3 (I)	Col4 (I)	Col5 (I)	Col6 (I)
User Header	User Row ID	T	t	V	R	D
1		30	0	10	100	-1
2		70	90	20	120	1



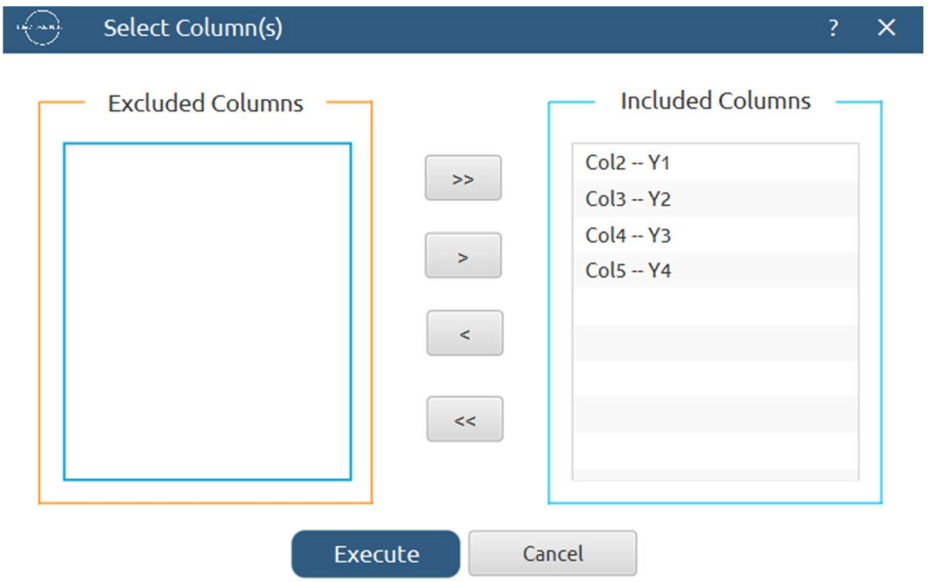
Results (right spreadsheet):

	Col1	Col2 (I)	Col3 (S)	Col4 (S)	Col5 (S)	Col6 (I)	Col7 (I)	Col8 (I)	Col9 (I)	Col10 (I)
User Header	User Row ID	Standard Order	Block Number	Replicate Number	Point Type	T	t	V	R	D
1		1	Block: 1	Replicate: 1	Design Point	30	90	10	100	-1
2		2	Block: 1	Replicate: 1	Design Point	70	30	10	100	1
3		3	Block: 1	Replicate: 1	Design Point	30	30	10	120	1
4		4	Block: 1	Replicate: 1	Design Point	30	30	20	120	1
5		5	Block: 1	Replicate: 1	Design Point	30	90	20	120	-1
6		6	Block: 1	Replicate: 1	Design Point	70	90	20	100	1
7		7	Block: 1	Replicate: 1	Design Point	70	90	10	120	1
8		8	Block: 1	Replicate: 1	Design Point	70	30	20	120	-1
9		9	Block: 1	Replicate: 1	Design Point	30	90	20	100	1
10		10	Block: 1	Replicate: 1	Design Point	70	90	10	120	-1
11		11	Block: 1	Replicate: 1	Design Point	70	30	20	100	-1
12		12	Block: 1	Replicate: 1	Design Point	30	30	10	100	-1

Step 2: Definition of response variables

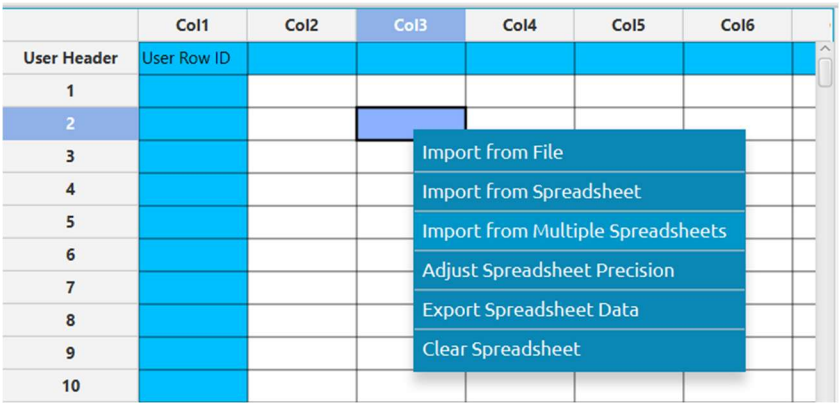
Create a new tab named “Responses” and define the responses in the column headers. Fill each column with the values of the corresponding responses that were observed and make sure the values follow the order of the experiments as given by the Plackett Burman method. Then, select all columns to be transferred to the right spreadsheet: *Data Transformation → Data Manipulation → Select Column(s)*

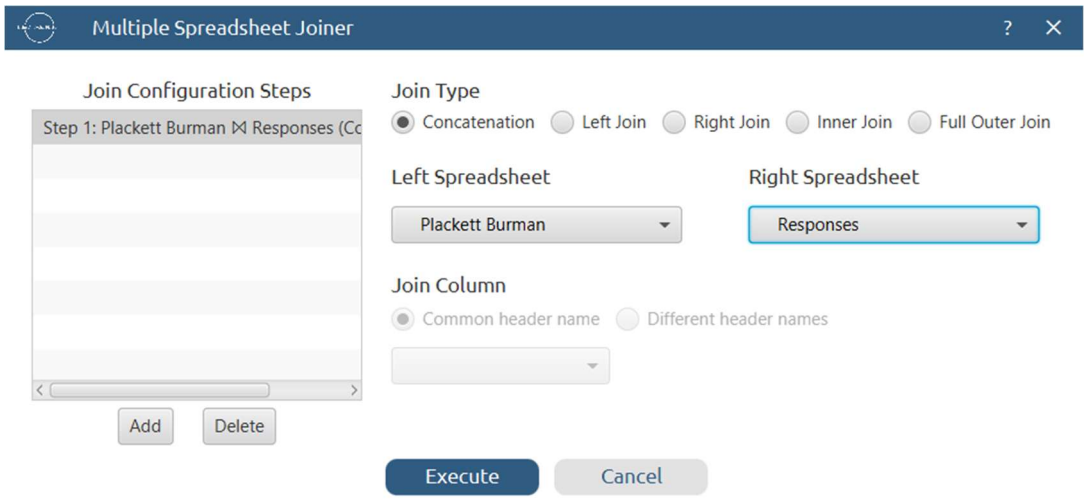
	Col1	Col2 (D)	Col3 (D)	Col4 (D)	Col5 (D)
User Header	User Row ID	Y1	Y2	Y3	Y4
1		10.3	20.4	12.6	43.3
2		54.1	26.75	13.5	94.4
3		8.1	18.3	12.6	39.1
4		7.6	25.1	12.9	45.6
5		9.7	21.3	12	43.9
6		56.3	31.1	15.4	102.8
7		61.5	27	14.3	102.8
8		56.6	26.6	15.4	98.6
9		9.5	17.7	13.8	40.9
10		60.5	27.4	15.4	103.3
11		45.8	26.4	14.1	86.2
12		9.6	19.5	12.6	41.7

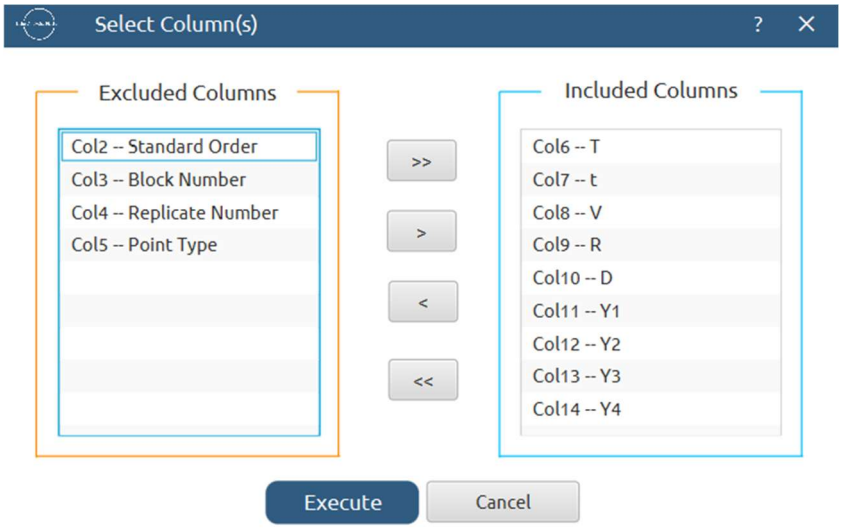


Step 3: Data isolation

Create a new tab named “Data” and import the results from the “Plackett Burman” and “Responses” spreadsheets by right clicking on the left spreadsheet. Then, select only the factors and responses columns to be transferred to the right spreadsheet: *Data Transformation → Data Manipulation → Select Column(s)*





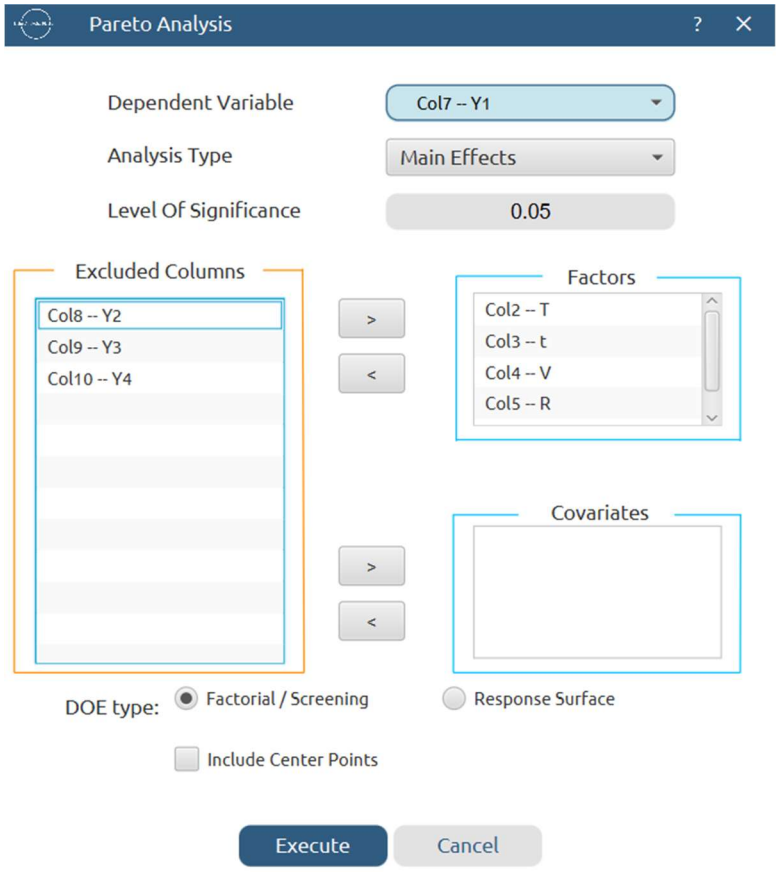


Results:

	Col1	Col2 (I)	Col3 (I)	Col4 (I)	Col5 (I)	Col6 (I)	Col7 (D)	Col8 (D)	Col9 (D)	Col10 (D)
User Header	User Row ID	T	t	V	R	D	Y1	Y2	Y3	Y4
1		30	90	10	100	-1	10.3	20.4	12.6	43.3
2		70	30	10	100	1	54.1	26.75	13.5	94.4
3		30	30	10	120	1	8.1	18.3	12.6	39.1
4		30	30	20	120	1	7.6	25.1	12.9	45.6
5		30	90	20	120	-1	9.7	21.3	12	43.9
6		70	90	20	100	1	56.3	31.1	15.4	102.8
7		70	90	10	120	1	61.5	27	14.3	102.8
8		70	30	20	120	-1	56.6	26.6	15.4	98.6
9		30	90	20	100	1	9.5	17.7	13.8	40.9
10		70	90	10	120	-1	60.5	27.4	15.4	103.3
11		70	30	20	100	-1	45.8	26.4	14.1	86.2
12		30	30	10	100	-1	9.6	19.5	12.6	41.7

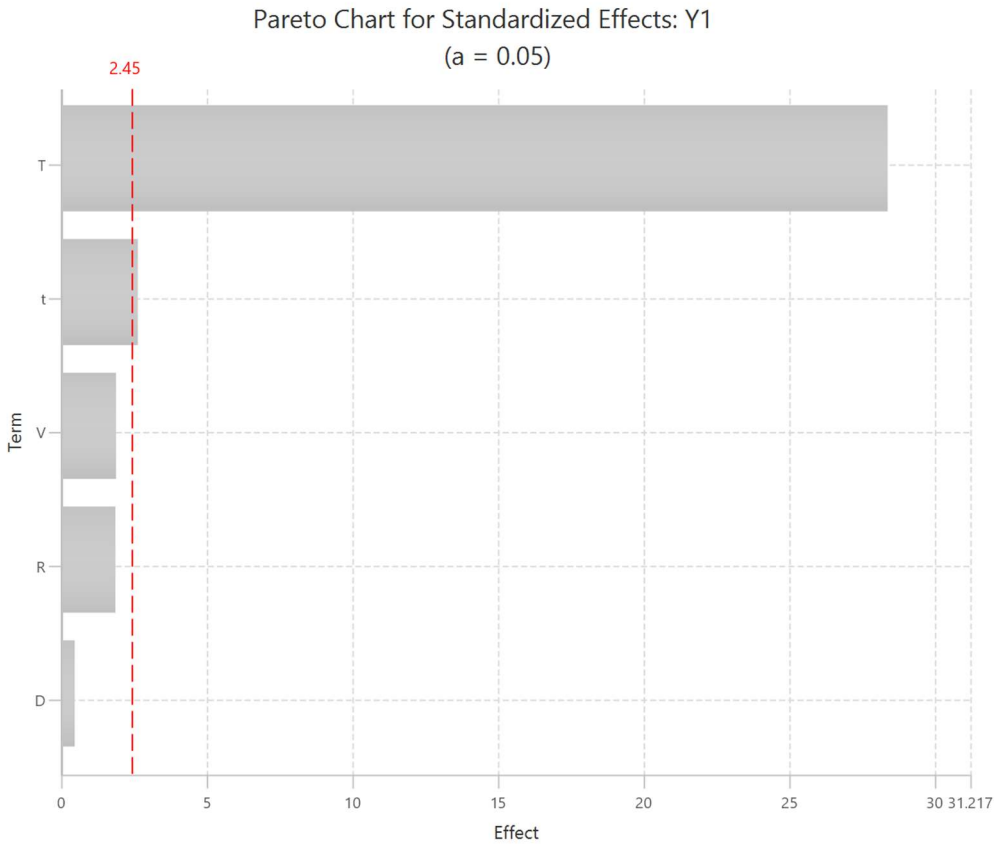
Step 4: Pareto analysis

Create a new tab named “Pareto Analysis – Y1” and import the results from the spreadsheet “Data”. Then, conduct pareto analysis for the first response variable, Y_1: *DOE → Post DoE Analysis → Pareto Analysis*



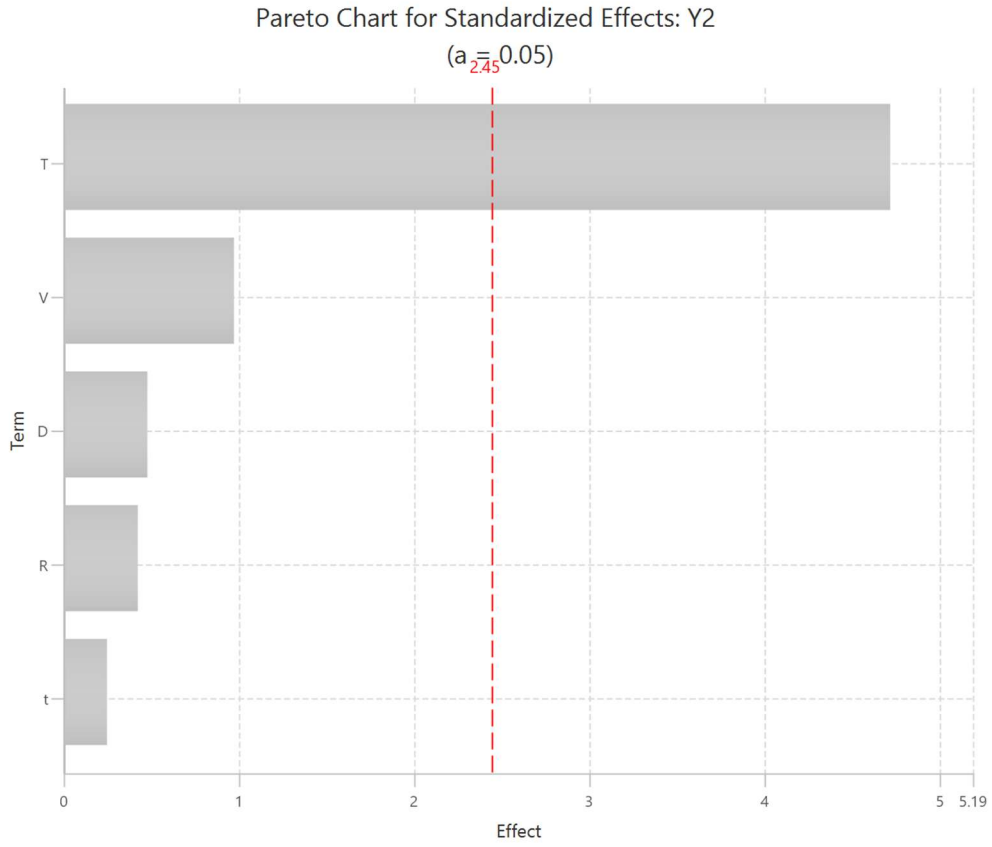
Results:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	28.3790262
3		t	2.6351953
4		V	1.8851782
5		R	1.8649074
6		D	0.4662269
7		Significance Value	2.4469119



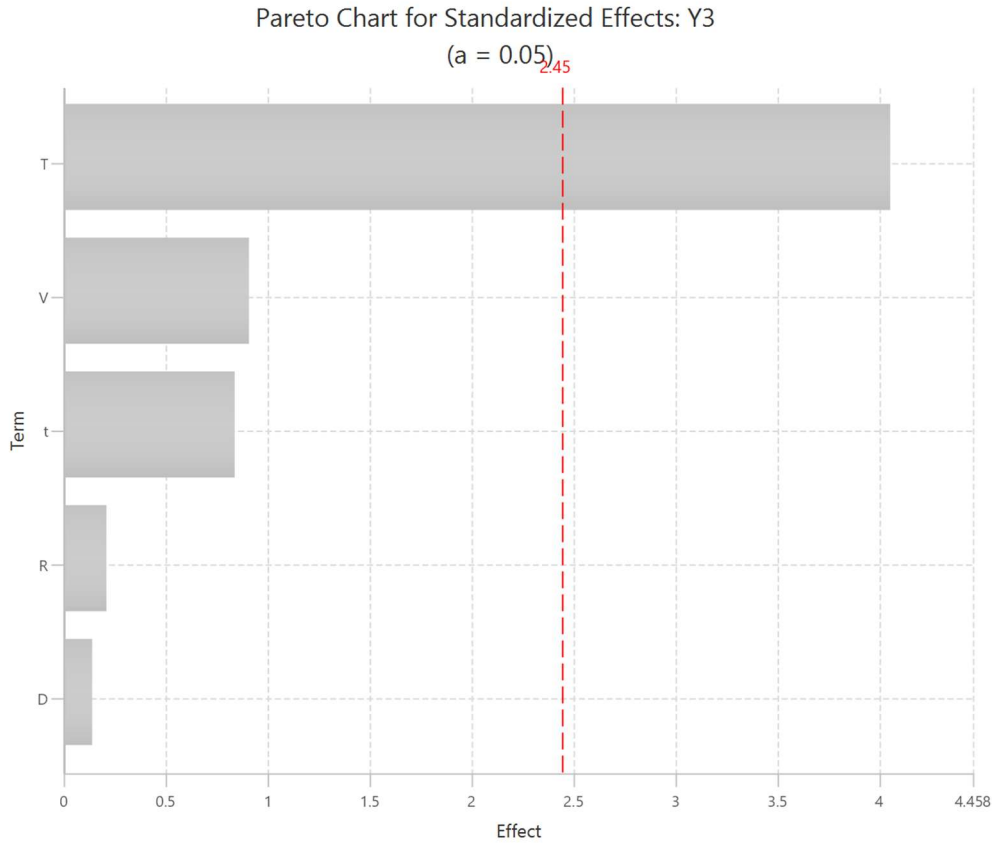
Repeat this step for the rest of the response variables. Results, Y_2:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	4.7178104
3		V	0.9721216
4		D	0.4778225
5		R	0.4229003
6		t	0.2471496
7		Significance Value	2.4469119



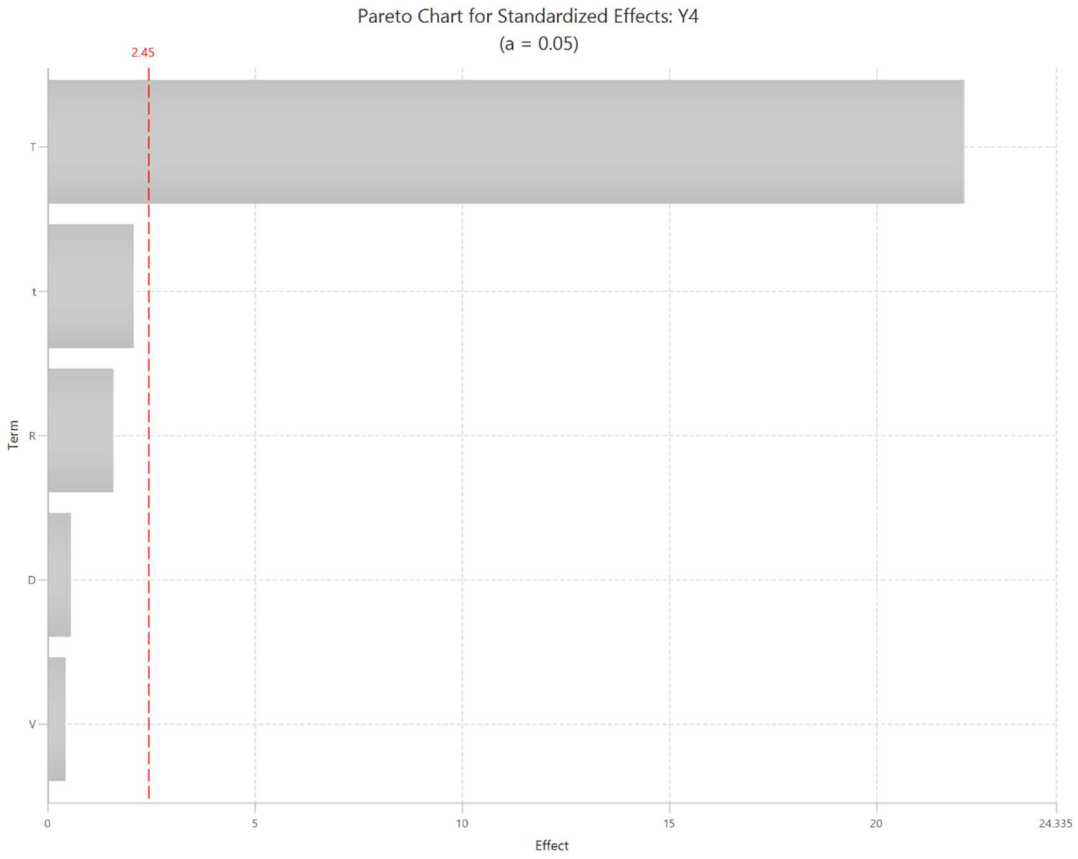
Results, Y_3:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	4.0525434
3		V	0.9083287
4		t	0.8384573
5		R	0.2096143
6		D	0.1397429
7		Significance Value	2.4469119



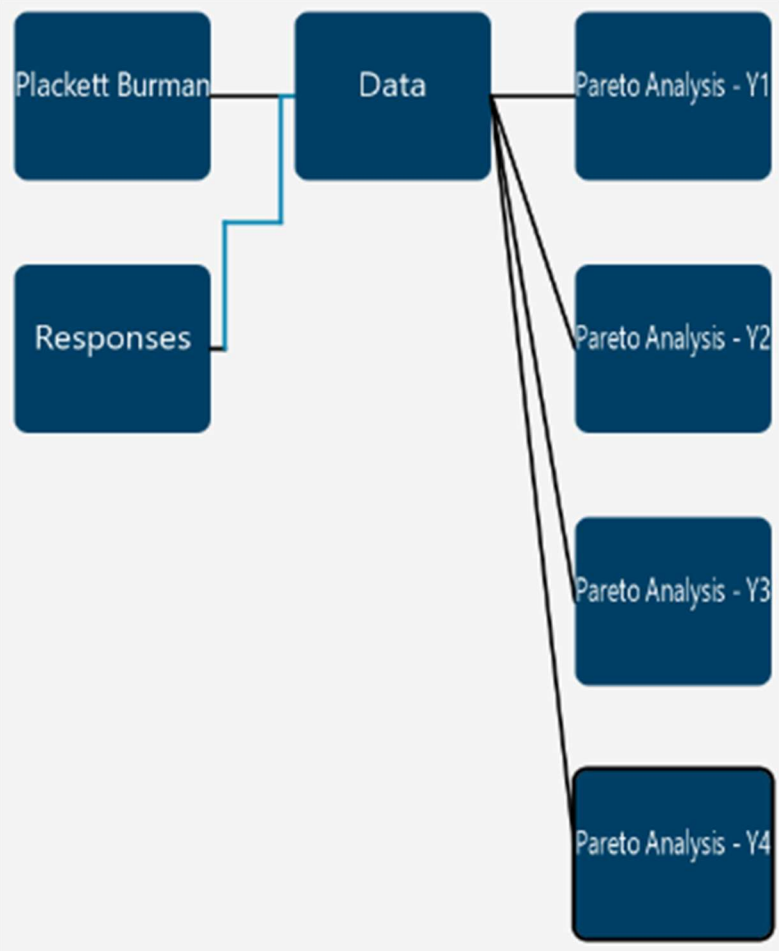
Results, Y_4:

	Col1	Col2 (S)	Col3 (S)
User Header	User Row ID	Pareto Analysis of :	Standardized Effects
1		Variable	Effect
2		T	22.1223272
3		t	2.0822574
4		R	1.5915343
5		D	0.5702998
6		V	0.4376719
7		Significance Value	2.4469119



Final Isalos Workflow

The final workflow is presented below:



References

(1) Ma, L.; Wang, L.; Tang, J.; Yang, Z. Optimization of Arsenic Extraction in Rice Samples by Plackett–Burman Design and Response Surface Methodology. *Food Chemistry* **2016**, *204*, 283–288. https://doi.org/10.1016/j.foodchem.2016.02.126.