

EDBO+ Tutorial

The screenshot shows the EDBO+ web application interface. At the top left is a sidebar with a logo, "Welcome to EDBO+", user icons, and a "Logout" button. The main area features a large logo with "EDBO+" and a subtitle: "Bayesian reaction optimization as a tool for chemical synthesis". Below this are four primary buttons: "Build" (green, highlighted with a red border), "Upload" (orange), "Delete" (red), and "Download" (blue). At the bottom is a blue button labeled "Optimize Reaction" with a share icon.

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EDBO+

Bayesian reaction optimization as a tool for chemical synthesis

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Step 1: In the homepage, click 'Build' to build the reaction scope.



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Introduce a name for your scope:

Suzuki_coupling_demo

Add model features:

Here we can generate a reaction scope by introducing the name of the features and the corresponding values that we would like to consider in our experiments. The **feature names** are the variables that we will study in your experiments and the **feature values** are the different states that we will consider for building our reaction scope. For instance, we can introduce a **temperature** feature with values **25.0, 30.0, 34.5** and a second feature **solvent** with values **DMSO, Water**. Use the **Add features** button to add as many features as you need for your scope. Note: Use **comma-separated** values to introduce the feature values.

Add Features

Create scope

Step 2: Fill in the name for your scope, and click 'add features'.



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Add model features:

Here we can generate a reaction scope by introducing the name of the features and the corresponding values that we would like to consider in our experiments. The **feature names** are the variables that we will study in your experiments and the **feature values** are the different states that we will consider for building our reaction scope. For instance, we can introduce a **temperature** feature with values **25.0, 30.0, 34.5** and a second feature **solvent** with values **DMSO, Water**. Use the **Add features** button to add as many features as you need for your scope. Note: Use **comma-separated** values to introduce the feature values.

[+ Add Features](#)

Ligand	L1, L2, L3, L4, L5, L6	Remove feature
Base	Na ₂ CO ₃ , K ₃ PO ₄ , Cs ₂ CO ₃ , NaOtBu	Remove feature
Solvent	THF, toluene, dioxane, DME	Remove feature
Temperature	60, 80, 100	Remove feature

[Create scope](#)

Step 3: Add a name for each feature and component (separated by comma). Click 'Create scope'.

Note: Do not use spaces (e.g. put Pd_equiv or Pd-equiv instead of Pd equiv). Avoid special characters such as parentheses.



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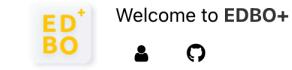
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Ligand	Base	Solvent	Temperature
L1	Na ₂ CO ₃	THF	60.0
L1	Na ₂ CO ₃	THF	80.0
L1	Na ₂ CO ₃	THF	100.0
L1	Na ₂ CO ₃	toluene	60.0
L1	Na ₂ CO ₃	toluene	80.0
L1	Na ₂ CO ₃	toluene	100.0
L1	Na ₂ CO ₃	dioxane	60.0
L1	Na ₂ CO ₃	dioxane	80.0
L1	Na ₂ CO ₃	dioxane	100.0
L1	Na ₂ CO ₃	DME	60.0
L1	Na ₂ CO ₃	DME	80.0
L1	Na ₂ CO ₃	DME	100.0
L1	K ₃ PO ₄	THF	60.0
L1	K ₃ PO ₄	THF	80.0
L1	K ₃ PO ₄	THF	100.0
L1	K ₃ PO ₄	toluene	60.0

The scope will be displayed. You can download the scope by clicking 'Download' on the left side of the screen.



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Optimize Reaction

Step 4: Go back to 'Home' and click 'Optimize Reaction'. You can also click 'Optimize' on the left side of the screen.



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Select an existing scope:

Suzuki_coupling_demo



[Setup Optimizer](#)

Step 5: Select the scope, and click 'Setup Optimizer'.



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Select the features for building the predictive model:

- Ligand
 - Base
 - Solvent
 - Temperature
- All selected (4)

- Search
- Select all
- Ligand
- Base
- Solvent
- Temperature

Select the optimization objectives:

Here you can add up to 3 objectives. Introduce in each objective whether it should be maximized or minimized during the optimization process. You can also introduce a minimum threshold for each objective (default is 0).

Select batch size:

Step 6: Select features for building the model. You can change the selections between rounds.



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Select the optimization objectives:

Here you can add up to 3 objectives. Introduce in each one the name of your targeted objective and whether this objective should be maximized or minimized during the optimization process. Also you can define a minimum threshold for each objective (default is None, no boundaries).

[+ Add Objectives](#)

Yield

Threshold

Maximize Minimize

[Remove](#)

Select batch size:

Number of experiments to run in parallel in the lab at each iteration. Note: you can change this value at each iteration step.

Step 7: Add objectives (yield, regioselectivity, ee, cost, etc.) and choose if the objective should be maximized or minimized. You can add up to 3 objectives. You can also add a threshold for each objective. For example, if you are only interested in reactions that give >80% ee, you can put a threshold to target specific search space.

Note: Make sure the spelling and letter case of the objective(s) are consistent across runs (i.e. you can't put "Yield" for round 1 and "yield" for round 2).



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Select batch size:

Number of experiments to run in parallel in the lab at each iteration. Note: you can change this value at each iteration step.

4

Run Optimizer

Step 8: Choose the number of experiments to run in parallel, and click 'Run Optimizer'.



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Next samples to collect:

Note: You can always download the entire scope here or in the [Download](#) section.

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Ligand	Base	Solvent	Temperature	Yield	priority
L3	K3PO4	THF	80.0	PENDING	1
L2	Cs2CO3	THF	80.0	PENDING	1
L2	NaOtBu	dioxane	80.0	PENDING	1
L5	K3PO4	DME	80.0	PENDING	1

[Download scope](#)

[Download predictions](#)

Step 9: Download the scope as .csv file.

Suzuki_coupling_demo — Saved to my Mac

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	Ligand	Base	Solvent	Temperature	Yield	priority																
2	L3	K3PO4	THF	80	36	1																
3	L2	Cs2CO3	THF	80	80	1																
4	L2	NaOtBu	dioxane	80	72	1																
5	L5	K3PO4	DME	80	57	1																
6	L5	K3PO4	DME	60	PENDING	0																
7	L4	NaOtBu	DME	80	PENDING	0																
8	L5	Na2CO3	toluene	60	PENDING	0																
9	L5	Na2CO3	THF	100	PENDING	0																
10	L5	Na2CO3	THF	80	PENDING	0																
11	L5	Na2CO3	THF	60	PENDING	0																
12	L4	NaOtBu	DME	100	PENDING	0																
13	L4	NaOtBu	DME	60	PENDING	0																
14	L5	Na2CO3	toluene	100	PENDING	0																
15	L4	NaOtBu	dioxane	100	PENDING	0																
16	L4	NaOtBu	dioxane	80	PENDING	0																
17	L4	NaOtBu	dioxane	60	PENDING	0																
18	L4	NaOtBu	toluene	100	PENDING	0																
19	L4	NaOtBu	toluene	80	PENDING	0																
20	L4	NaOtBu	toluene	60	PENDING	0																
21	L5	Na2CO3	toluene	80	PENDING	0																
22	L5	Na2CO3	dioxane	60	PENDING	0																
23	L5	K3PO4	dioxane	100	PENDING	0																
24	L5	Na2CO3	dioxane	80	PENDING	0																

Step 10: Perform the experiments with priority = 1, and input the yield results in the .csv file. Save it as a .csv file.



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Build



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Delete



Download



Optimize Reaction

Step 11: Go back to 'Home' and click 'Upload'. You can also click 'Upload' on the left side of the screen.



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Name of the scope to be uploaded:

Here you can upload your .csv, .xls or .xlsx file containing the reaction scope.

Suzuki_coupling_demo_round_0



Choose an existing scope file...



Upload

Step 12: Open the scope file, and click 'Upload'



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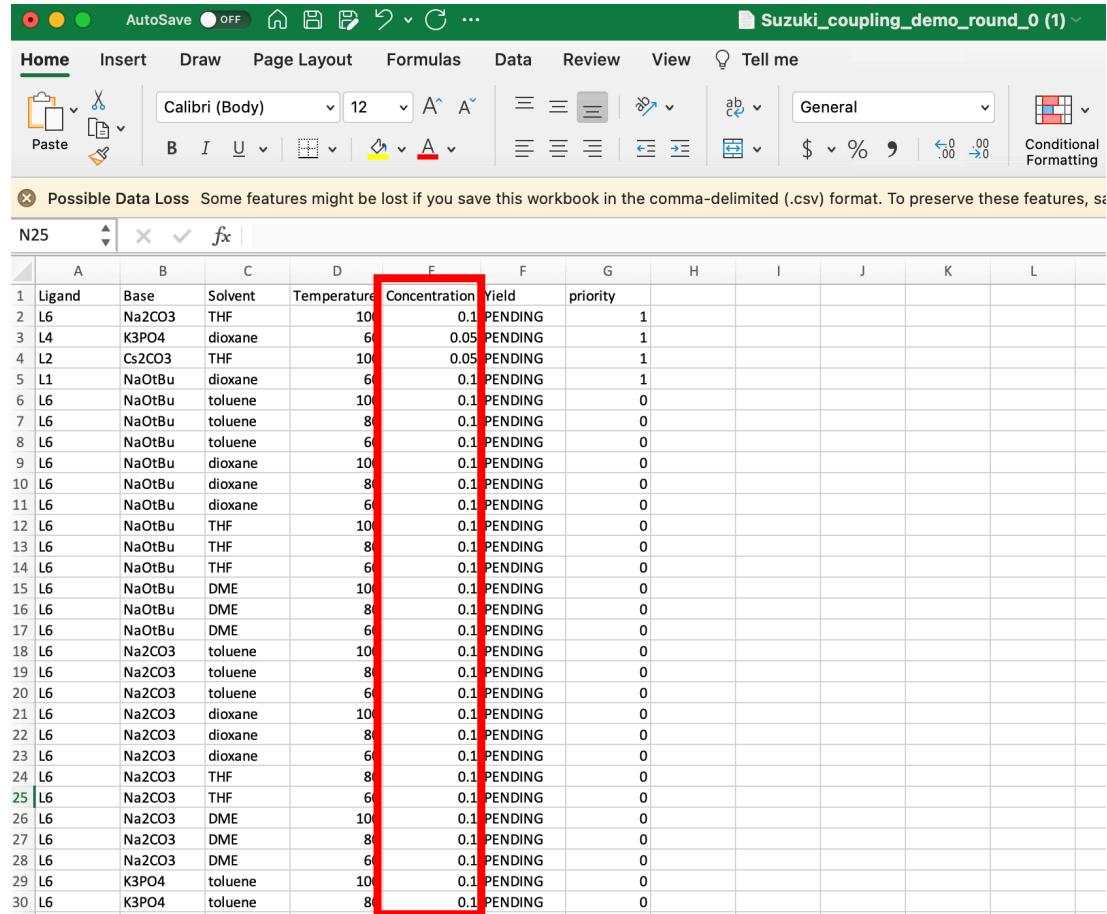
Select an existing scope:

Suzuki_coupling_demo_round_0 ▾

Setup Optimizer

Step 13: Repeat Step 5 to 12 but with the updated scope. Iterate the process until the desired goal is achieved.

How to modify scope

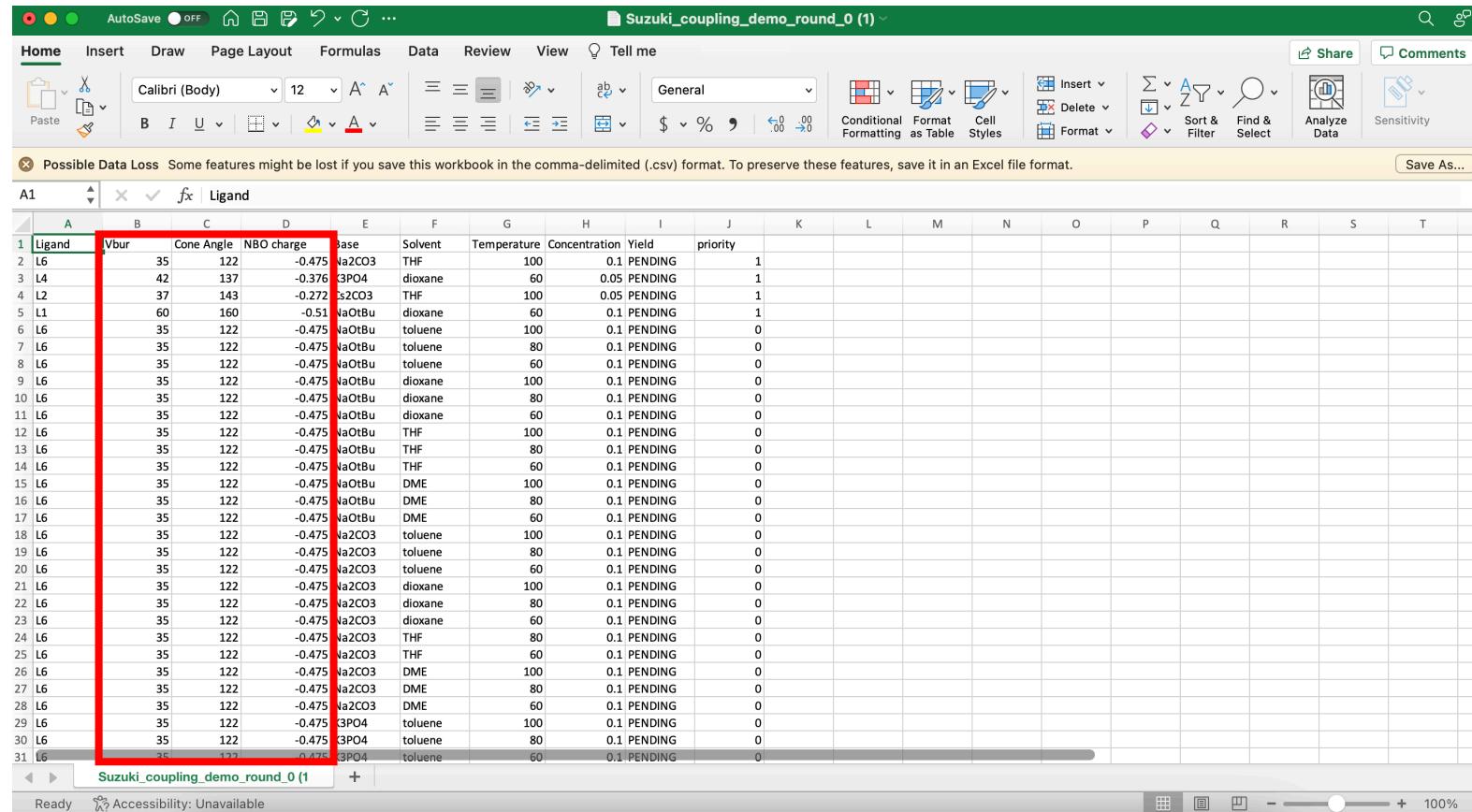


The screenshot shows a Microsoft Excel spreadsheet titled "Suzuki_coupling_demo_round_0 (1)". The table has columns labeled Ligand, Base, Solvent, Temperature, Concentration, Yield, and priority. The "Concentration" column is highlighted with a red box. The data consists of 30 rows of experimental runs, each with a unique ID (L1-L6) and various reaction conditions.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Ligand	Base	Solvent	Temperature	Concentration	Yield	priority					
2	L6	Na2CO3	THF	100	0.1	PENDING	1					
3	L4	K3PO4	dioxane	6	0.05	PENDING	1					
4	L2	Cs2CO3	THF	100	0.05	PENDING	1					
5	L1	NaOtBu	dioxane	6	0.1	PENDING	1					
6	L6	NaOtBu	toluene	100	0.1	PENDING	0					
7	L6	NaOtBu	toluene	80	0.1	PENDING	0					
8	L6	NaOtBu	toluene	60	0.1	PENDING	0					
9	L6	NaOtBu	dioxane	100	0.1	PENDING	0					
10	L6	NaOtBu	dioxane	80	0.1	PENDING	0					
11	L6	NaOtBu	dioxane	60	0.1	PENDING	0					
12	L6	NaOtBu	THF	100	0.1	PENDING	0					
13	L6	NaOtBu	THF	80	0.1	PENDING	0					
14	L6	NaOtBu	THF	60	0.1	PENDING	0					
15	L6	NaOtBu	DME	100	0.1	PENDING	0					
16	L6	NaOtBu	DME	80	0.1	PENDING	0					
17	L6	NaOtBu	DME	60	0.1	PENDING	0					
18	L6	Na2CO3	toluene	100	0.1	PENDING	0					
19	L6	Na2CO3	toluene	80	0.1	PENDING	0					
20	L6	Na2CO3	toluene	60	0.1	PENDING	0					
21	L6	Na2CO3	dioxane	100	0.1	PENDING	0					
22	L6	Na2CO3	dioxane	80	0.1	PENDING	0					
23	L6	Na2CO3	dioxane	60	0.1	PENDING	0					
24	L6	Na2CO3	THF	80	0.1	PENDING	0					
25	L6	Na2CO3	THF	60	0.1	PENDING	0					
26	L6	Na2CO3	DME	100	0.1	PENDING	0					
27	L6	Na2CO3	DME	80	0.1	PENDING	0					
28	L6	Na2CO3	DME	60	0.1	PENDING	0					
29	L6	K3PO4	toluene	100	0.1	PENDING	0					
30	L6	K3PO4	toluene	80	0.1	PENDING	0					

You can update the scope during the optimization campaign without losing any progress. For example, you can add a new variable (concentration) that can alter the reaction yield, or remove a ligand that consistently gave no yield. To modify your scope, build a new scope including the new feature/component. Once you have downloaded the .csv file, include the experimentally obtained objective(s) from previous iterations.

How to add features for discrete variables



Ligand	%Vbur	Cone Angle	NBO charge	base	Solvent	Temperature	Concentration	Yield	priority
L6	35	122	-0.475	Na2CO3	THF	100	0.1	PENDING	1
L4	42	137	-0.376	K3PO4	dioxane	60	0.05	PENDING	1
L2	37	143	-0.272	Li2CO3	THF	100	0.05	PENDING	1
L1	60	160	-0.51	NaOtBu	dioxane	60	0.1	PENDING	1
L6	35	122	-0.475	NaOtBu	toluene	100	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	toluene	80	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	toluene	60	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	dioxane	100	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	dioxane	80	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	dioxane	60	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	THF	100	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	THF	80	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	THF	60	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	DME	100	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	DME	80	0.1	PENDING	0
L6	35	122	-0.475	NaOtBu	DME	60	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	toluene	100	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	toluene	80	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	toluene	60	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	dioxane	100	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	dioxane	80	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	dioxane	60	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	THF	80	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	THF	60	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	DME	100	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	DME	80	0.1	PENDING	0
L6	35	122	-0.475	Na2CO3	DME	60	0.1	PENDING	0
L6	35	122	-0.475	K3PO4	toluene	100	0.1	PENDING	0
L6	35	122	-0.475	K3PO4	toluene	80	0.1	PENDING	0
L6	35	122	-0.475	K3PO4	toluene	60	0.1	PENDING	0

To include features, you will need to explicitly define the features for each component. In this example, we want to include '%Vbur', 'cone angle', and 'NBO charge' for the ligands in the scope. Begin by building the scope in the query builder listing out the ligands. Once you have downloaded the .csv file, you can add in a new column for each feature. Make sure these features match the ligand listed in the ligand column.



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Select the features for building the predictive model:

Ligand

Vbur

ConeAngle

NBOcharge

7 selected

Search

Select all

Ligand

Vbur

ConeAngle

NBOcharge

Base

Solvent

Temperature

Concentration

Select the optimization objectives:

Here you can add up to 3 objectives. Introduce in each row the name of the objective, whether it should be maximized or minimized during the optimization process and the minimum threshold for each objective (default is 0).

Select batch size:

Number of experiments to run in parallel in the next iteration step. You can change this value at each iteration step.

When selecting features, include all features except the variable itself, in this case 'Ligand'.

How to visualize data

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Next samples to collect:

Note: You can always download the entire scope here or in the **Download** section.

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Ligand	Base	Solvent	Temperature	Yield	priority
L5	Cs ₂ CO ₃	dioxane	60	PENDING	1.0
L4	K ₃ PO ₄	toluene	100	PENDING	1.0
L3	NaOtBu	THF	60	PENDING	1.0
L2	NaOtBu	dioxane	100	PENDING	1.0

 Download scope

 Download predictions

Download predictions as .csv file.

AutoSave OFF

pred_Suzuki_coupling_demo_round_0

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Paste Calibri (Body) 12 A⁺ A⁻ Wrap Text General Conditional Formatting as Table Sort & Filter Insert Format Cell Styles Analyze Data Sensitivity

Yield_predicted_mean

G1

Ligand **Base** **Solvent** **Temperature** **Yield** **priority** **Yield_predicted_mean** **Yield_predicted_variance** **Yield_expected_improvement**

1 L5 Cs2CO3 dioxane 60 PENDING 69.46450472 112.7740807 80.91643895

2 L4 K3PO4 toluene 100 PENDING 69.02999651 112.774135 80.91199258

3 L3 NaOtBu THF 60 PENDING 69.02999651 112.7740893 80.91199327

4 L2 NaOtBu dioxane 100 PENDING 68.69538732 112.7740689 80.92100134

5 L6 NaOtBu toluene 100 PENDING 68.63904377 112.7741544 80.91651788

6 L6 NaOtBu toluene 80 PENDING 68.59710963 24.73228789 12.44385288

7 L6 NaOtBu toluene 60 PENDING 68.59710963 112.7741544 80.91651788

8 L6 NaOtBu dioxane 100 PENDING 68.3529929 112.7741218 80.91698898

9 L6 NaOtBu dioxane 80 PENDING 68.20613848 19.91605358 9.109368401

10 L6 NaOtBu dioxane 60 PENDING 68.20613848 112.7741218 80.91698898

11 L6 NaOtBu THF 100 PENDING 67.90414031 112.774112 80.91605077

12 L6 NaOtBu THF 80 PENDING 67.82596374 19.84868102 8.68825448

13 L6 NaOtBu THF 60 PENDING 64.02811561 112.774112 80.91605077

14 L6 NaOtBu DME 100 PENDING 63.86492446 112.7741095 80.91648458

15 L6 NaOtBu DME 80 PENDING 63.86492446 19.45654288 8.572956168

16 L6 NaOtBu DME 60 PENDING 63.86331913 112.7741095 80.91648458

17 L6 Na2CO3 toluene 100 PENDING 63.40663875 112.7741836 80.91605392

18 L6 Na2CO3 toluene 80 PENDING 63.40663875 28.06622637 14.72778353

19 L6 Na2CO3 toluene 60 PENDING 63.40663875 112.7741836 80.91605392

20 L6 Na2CO3 dioxane 100 PENDING 63.27248521 112.7741544 80.91651788

21 L6 Na2CO3 dioxane 80 PENDING 63.27248521 24.73228789 12.44385288

22 L6 Na2CO3 dioxane 60 PENDING 63.27248521 112.7741544 80.91651788

23 L6 Na2CO3 THF 100 PENDING 63.27248521 112.7741399 80.9155853

24 L6 Na2CO3 THF 80 PENDING 63.27248521 22.69367458 10.5523655

25 L6 Na2CO3 THF 60 PENDING 63.27248521 112.7741399 80.9155853

26 L6 Na2CO3 DME 100 PENDING 63.26412412 112.7741392 80.91601616

27 L6 Na2CO3 DME 80 PENDING 63.26412412 23.0723523 11.00108837

28 L6 Na2CO3 DME 60 PENDING 63.15365219 112.7741392 80.91601616

29 L6 K3PO4 toluene 100 PENDING 63.15365219 112.774135 80.91199258

30 L6 K3PO4 toluene 80 PENDING 63.15365219 21.77327513 8.355411486

31 L6 K3PO4 toluene 60 PENDING 63.15365219 112.774135 80.91199258

32 L6 K3PO4 toluene 40 PENDING 63.14449320 112.7741072 80.91244054

Average: 61.32438623 Count: 289 Sum: 17661.42323

Ready Accessibility: Unavailable 100%

Predicted objective mean, variance, and expected improvement (referring to uncertainties) are provided in the prediction file. You can sort and plot the data.