Walkthrough of the Bayesian Optimization Interface

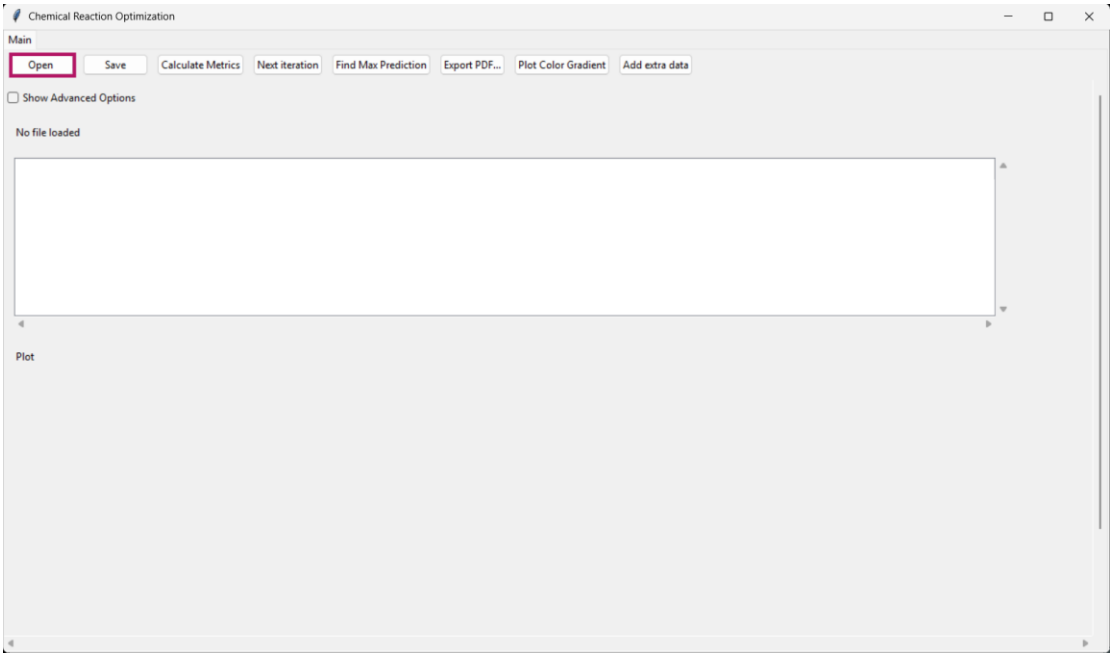
System Requirements

The graphical interface is designed to operate on **Microsoft Windows**.
Users wishing to deploy the application under **Linux** or **macOS** should do so through a **Windows-compatible execution layer** (e.g., *Wine*) or a **Windows virtual machine**.

1. Loading the Dataset

Upon launching the program, the interface opens on the **Main** tab.
To initialize a session, select the dataset using the **"Open"** button.
The program then automatically displays:

- the **initial reaction conditions** associated with **substrate 8**, and
- the corresponding **measured outputs** present in the file.



Entry	n moles	acid mass (g)	amine mass (g)	temperature (°C)	time (min)	conversion (%)	productivity (g/day)	PMI	Target
1	0.004343	1	1	210	60	60	20.89	2.30	2.94
2	0.001718	0.396	1.604	245	87	85	8.06	4.11	2.69
3	0.004343	1	1	210	90	60	13.92	2.30	2.94
4	0.001718	0.396	1.604	245	40	85	17.53	4.11	2.69
5	0.005646	1.3	0.7	210	34	61	48.55	1.74	3.82

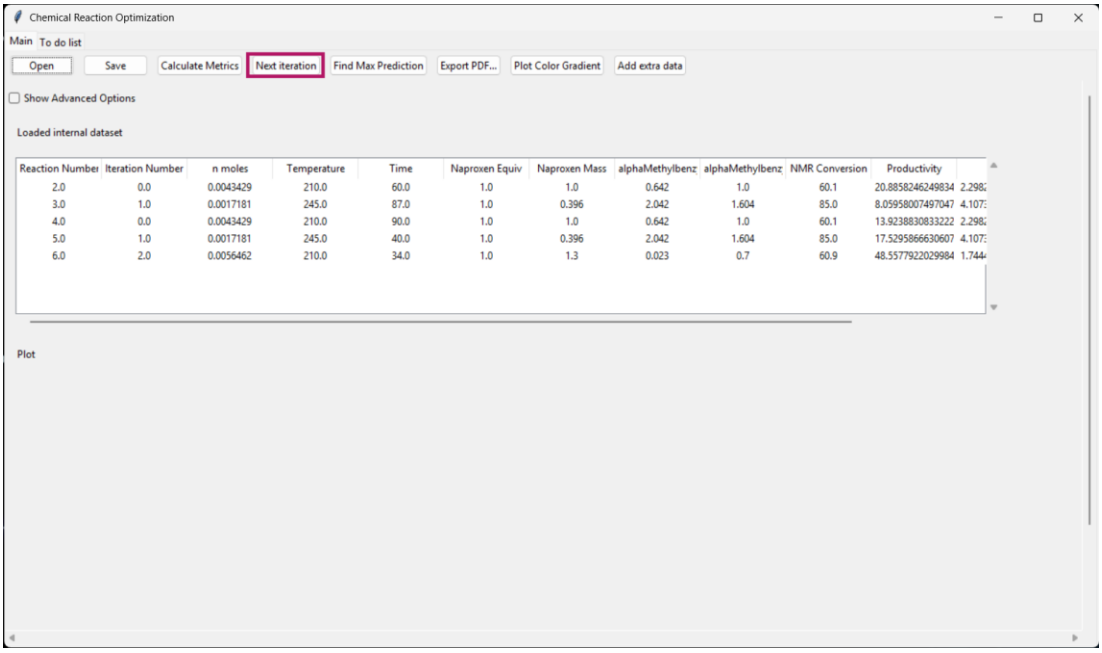
2. Initiating Bayesian Optimization

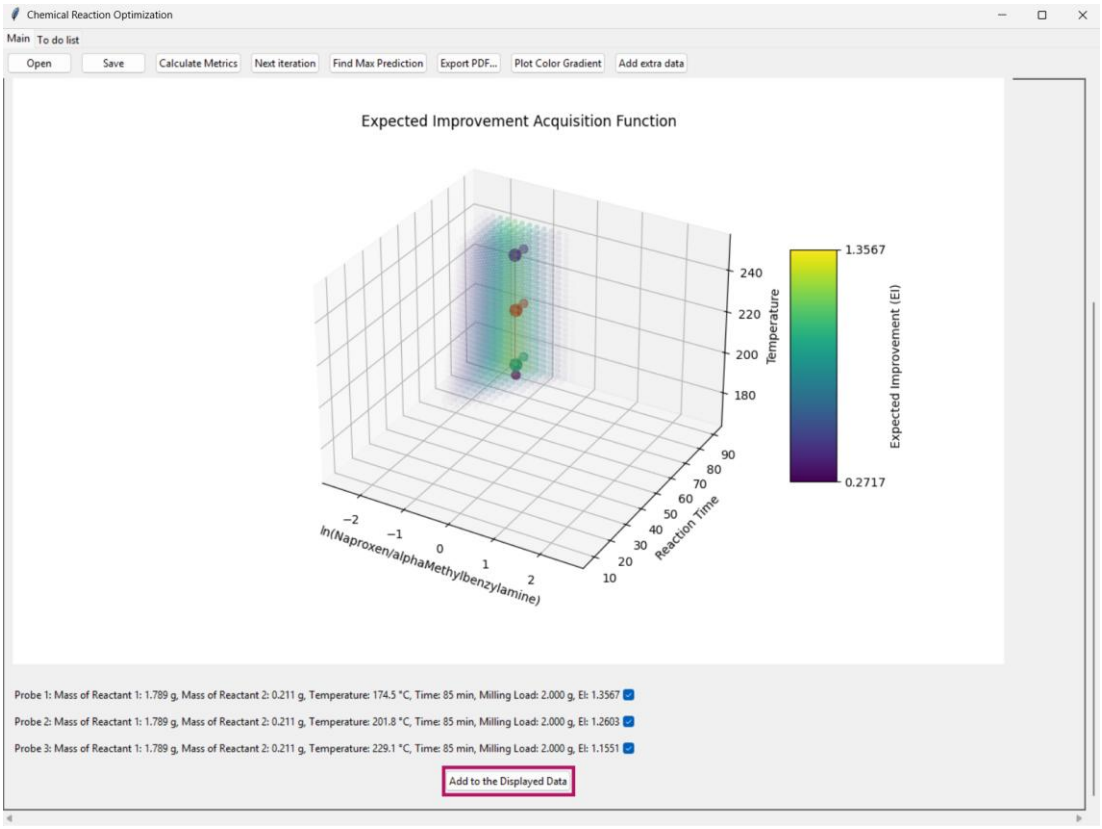
The next iteration of Bayesian optimization can be generated by selecting **“Next iteration.”**

At each iteration, the software:

- trains a Gaussian Process surrogate model,
- evaluates candidate experiments using the **Tempered Expected Improvement (TEI)** acquisition function,
- displays the **three suggested experimental probes** with their associated TEI values below the plot.

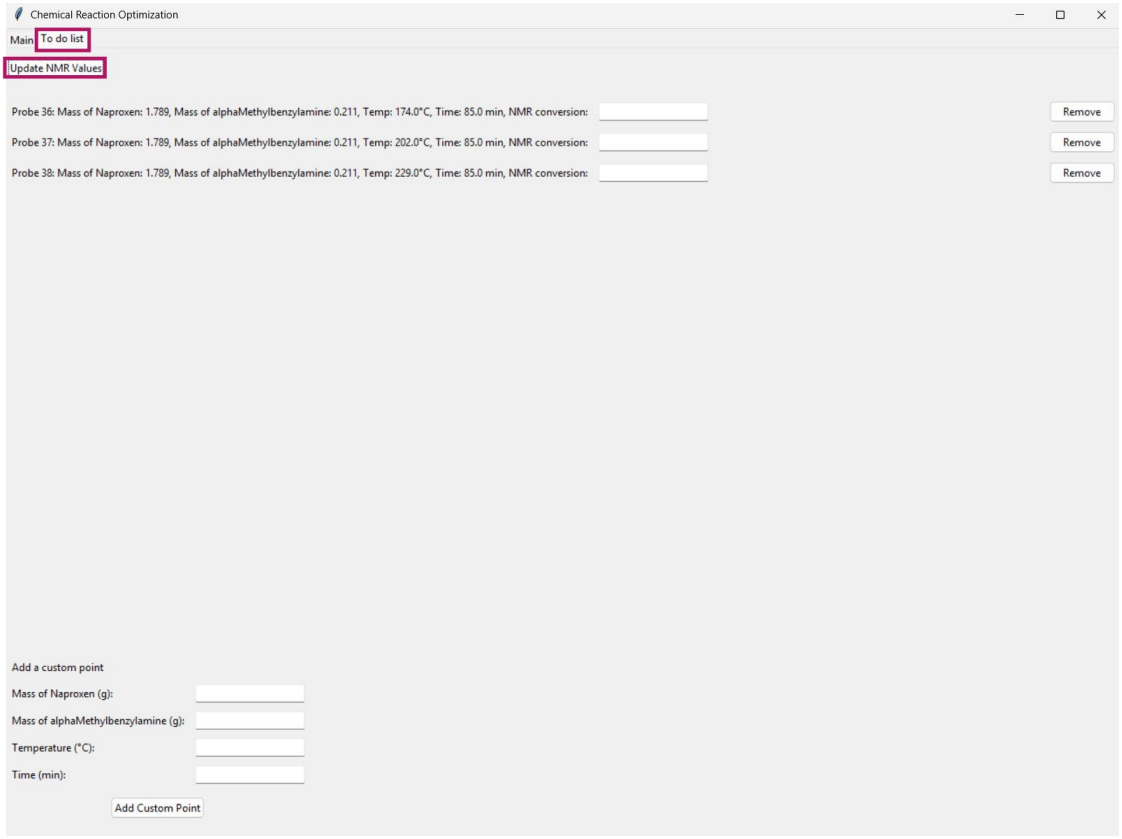
To register these proposed experiments as pending measurements, select **“Add to the displayed data.”**
This action unlocks the **“To do list”** tab, where experimental results can later be entered.




Chemical Reaction Optimization
Main
To do list
Open
Save
Calculate Metrics
Next iteration
Find Max Prediction
Export PDF...
Plot Color Gradient
Add extra data
Expected Improvement Acquisition Function
ln(Naproxen/alphaMethylbenzylamine)
Reaction Time
Temperature
Expected Improvement (EI)
1.3567
0.2717
Probe 1: Mass of Reactant 1: 1.789 g, Mass of Reactant 2: 0.211 g, Temperature: 174.5 °C, Time: 85 min, Milling Load: 2.000 g, EI: 1.3567
Probe 2: Mass of Reactant 1: 1.789 g, Mass of Reactant 2: 0.211 g, Temperature: 201.8 °C, Time: 85 min, Milling Load: 2.000 g, EI: 1.2603
Probe 3: Mass of Reactant 1: 1.789 g, Mass of Reactant 2: 0.211 g, Temperature: 229.1 °C, Time: 85 min, Milling Load: 2.000 g, EI: 1.1551
Add to the Displayed Data

3. Recording Experimental Outcomes

In the **To do list** tab, users may input the **experimental conversion values** obtained for the recommended reactions.
Once the new data are entered, selecting **"Update NMR Values"** commits them to the dataset and updates the model.
The user may then return to the **Main** tab to generate the next optimization iteration.



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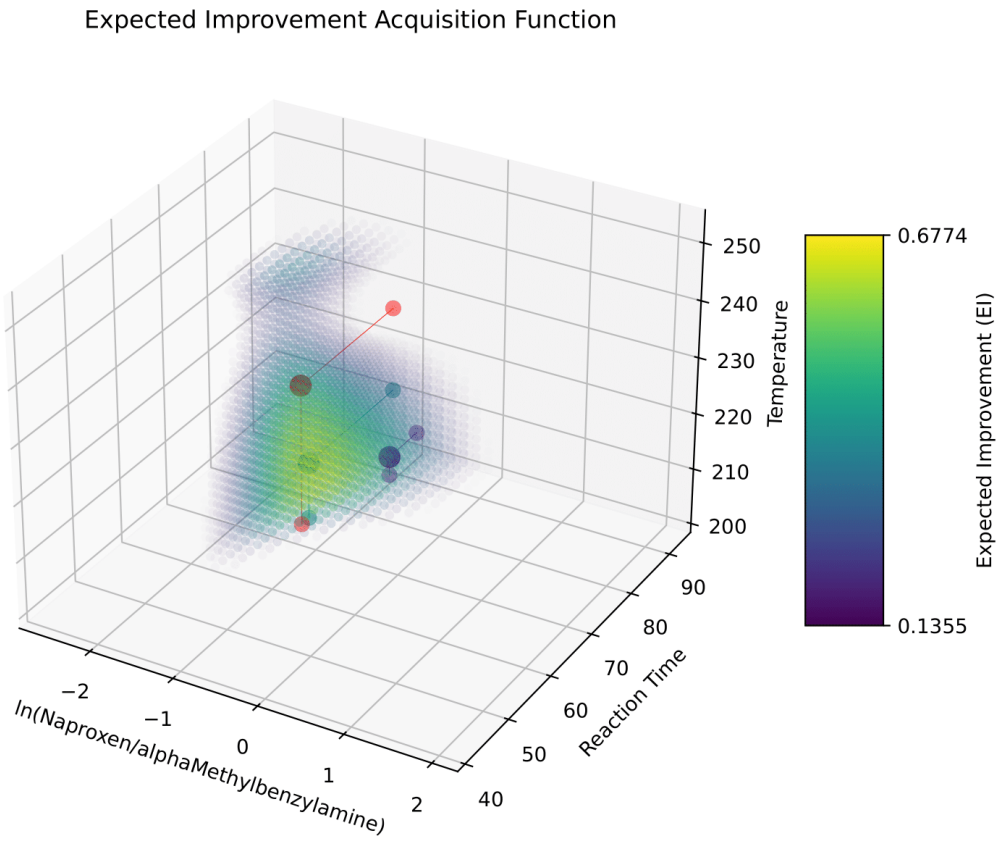
5	0.005646	1.3	0.7	210	34	61	48.55	1.74	3.82
6	0.001745	1.789	0.211	174	85	45	4.44	7.64	0.89
7	0.001745	1.789	0.211	202	85	99	9.76	3.47	4.22
8	0.001745	1.789	0.211	229	85	100	9.86	3.44	4.33

4. Optimization Progression

Typical progression consists of a sequence of iterations (e.g., Iterations 2–5), during which the model converges toward a region of maximum reactivity.
The reaction space narrows as new conversion values are provided, refining the Gaussian Process predictions and TEI landscape.

Iteration 2



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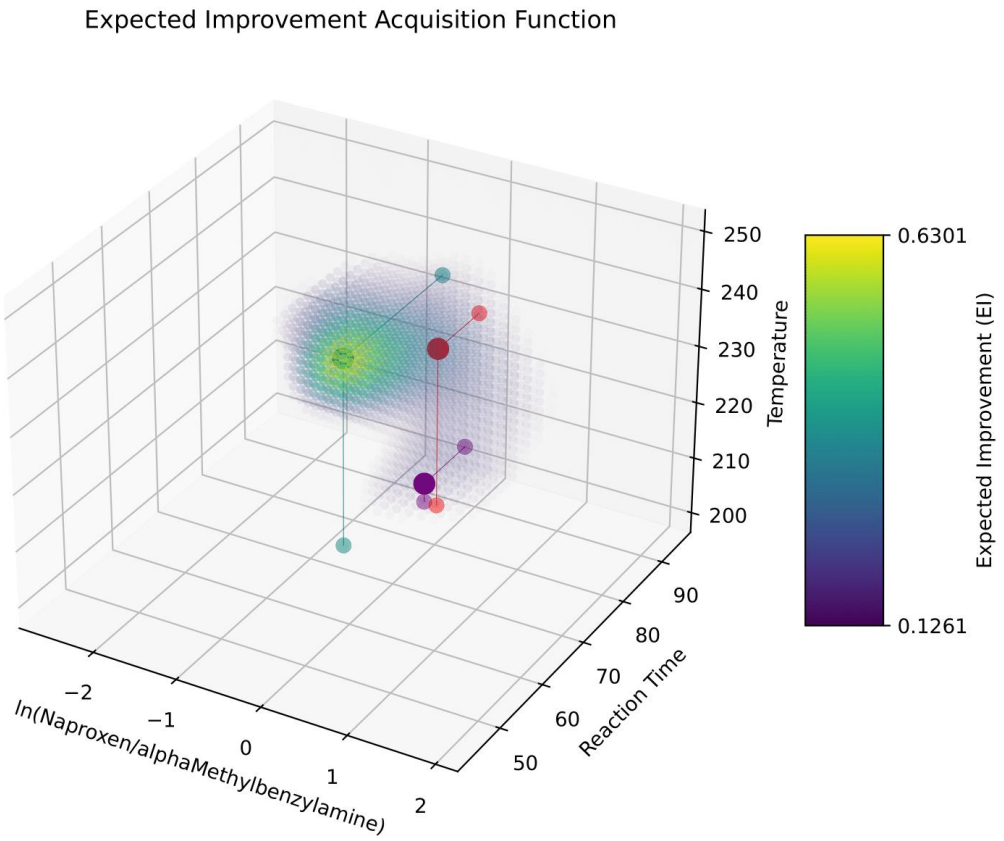
9	0.002278	1.724	0.276	212	72	100	15.19	2.63	4.89
10	0.002278	1.724	0.276	227	70	100	15.62	2.63	4.89
11	0.002933	1.644	0.356	205	85	100	16.57	2.05	5.58

Iteration 3



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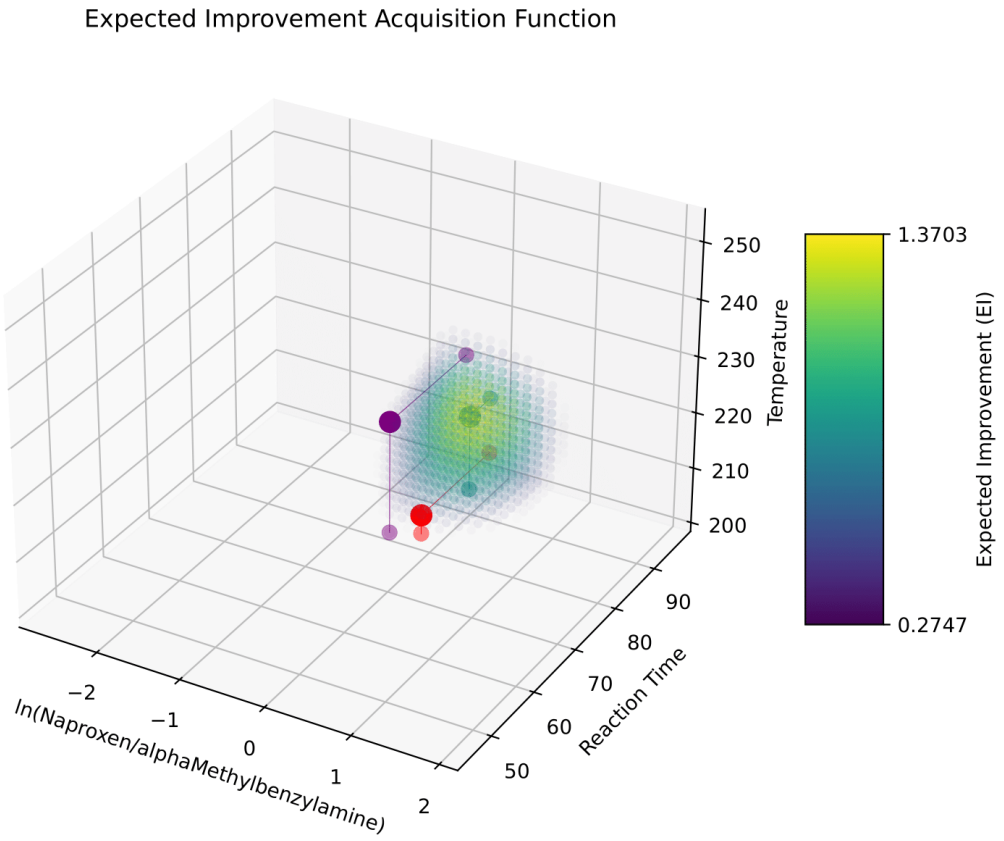
12	0.003616	1.562	0.438	233	71	100	24.45	1.66	6.30
13	0.005043	1.389	0.611	228	84	78	22.48	1.52	4.87
14	0.004533	1.451	0.549	203	84	82	21.25	1.61	4.86

Iteration 4



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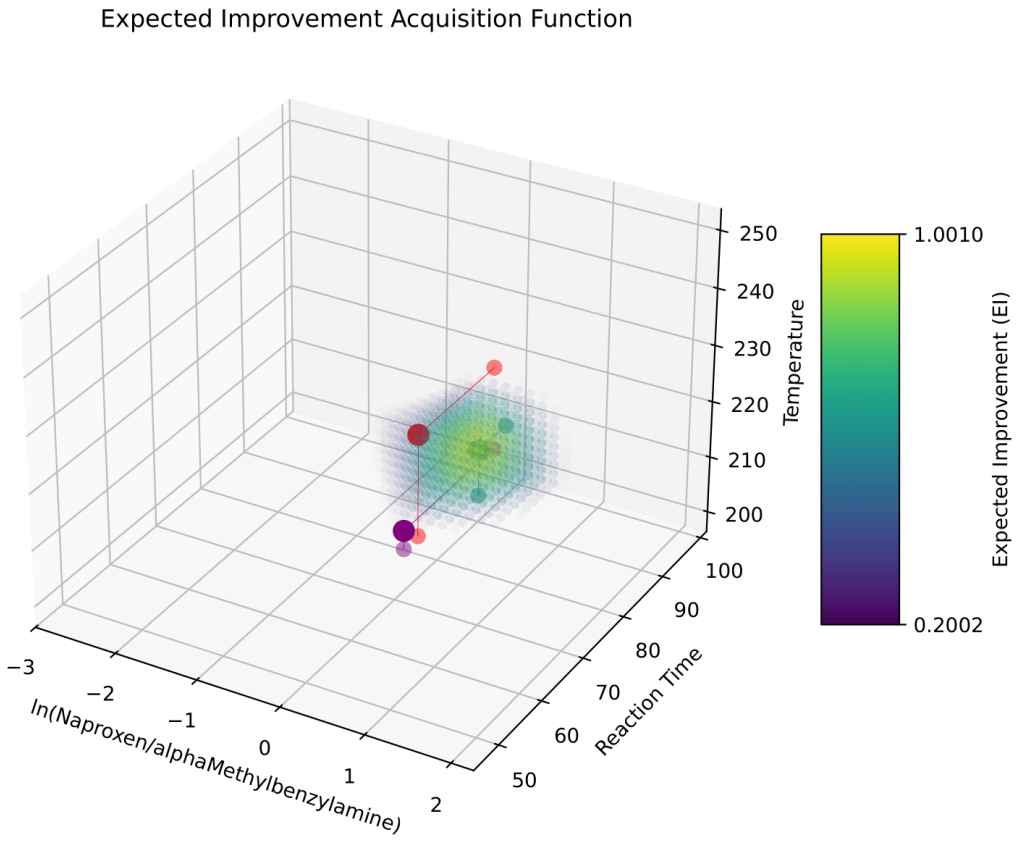
14	0.004533	1.451	0.549	203	84	82	21.25	1.61	4.86
15	0.005429	1.342	0.658	215	91	80	22.92	1.38	5.40
16	0.005429	1.342	0.658	205	79	76	25.08	1.45	4.97
17	0.004397	1.467	0.533	222	78	96	25.98	1.42	6.54

Iteration 5



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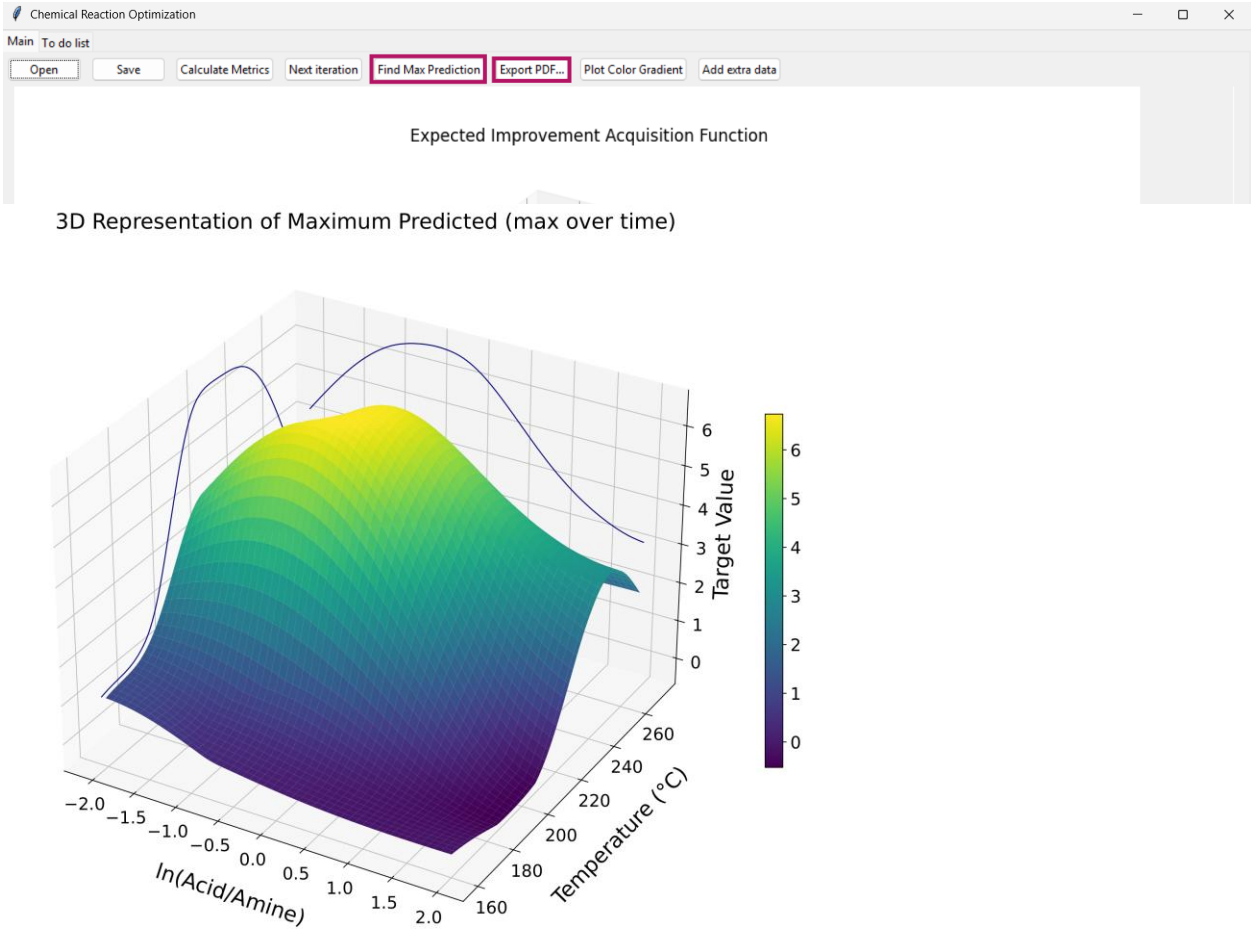
17	0.004397	1.467	0.533	222	78	96	25.98	1.42	6.54
18	0.005451	1.339	0.661	208	91	79	22.72	1.39	5.31
19	0.004908	1.405	0.595	218	80				
20	0.004908	1.405	0.595	203	76				

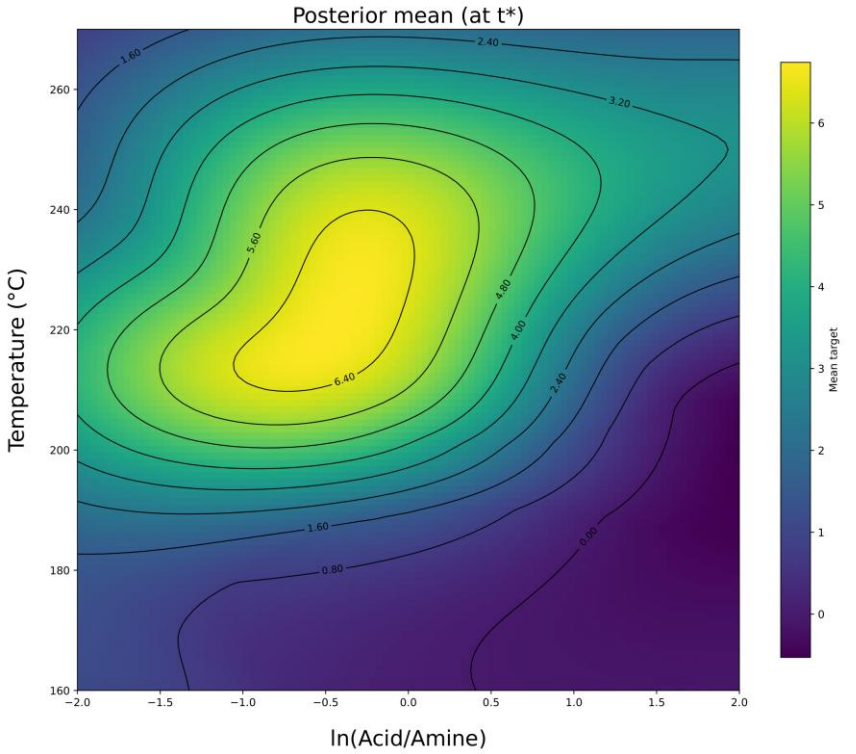
5. Termination and Export

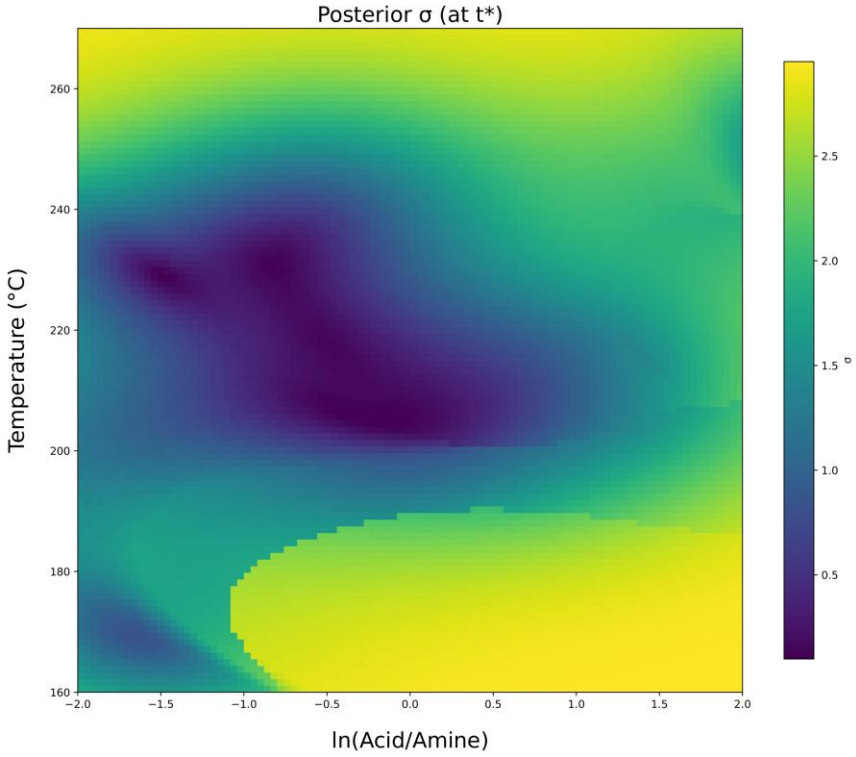
Optimization may be halted once the target surface becomes sufficiently explored, typically upon stabilizing near the optimum (e.g., around **experiments 12–17**).
Alternatively, additional experiments may be performed until available reagents are exhausted.

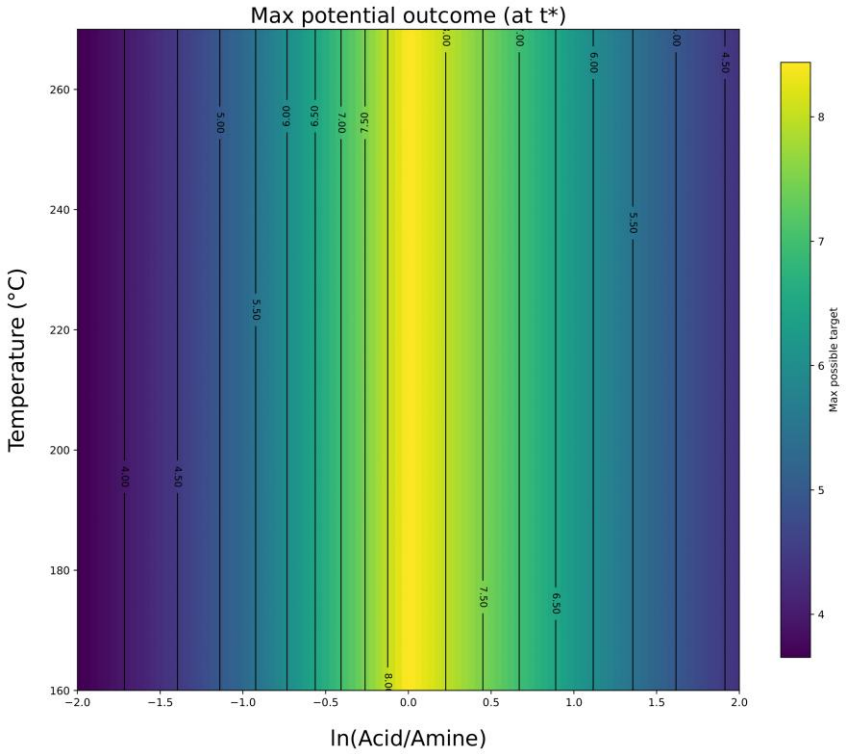
Upon completion:

- The **best predicted reaction conditions** can be extracted with **“Find max prediction.”**
- All plots generated during the optimization campaign can be exported using **“Export PDF.”**




Posterior mean (at t*)
Temperature (°C)
ln(Acid/Amine)
Mean target
1.60
2.40
3.20
5.60
4.80
4.00
6.40
2.40
1.60
0.80
0.00


Posterior σ (at t*)
Temperature (°C)
ln(Acid/Amine)
σ


Max potential outcome (at t*)
Temperature (°C)
ln(Acid/Amine)
Max possible target
160
180
200
220
240
260
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
4
5
6
7
8
4.00
4.50
5.00
5.50
6.00
6.50
7.00
7.50
8.00