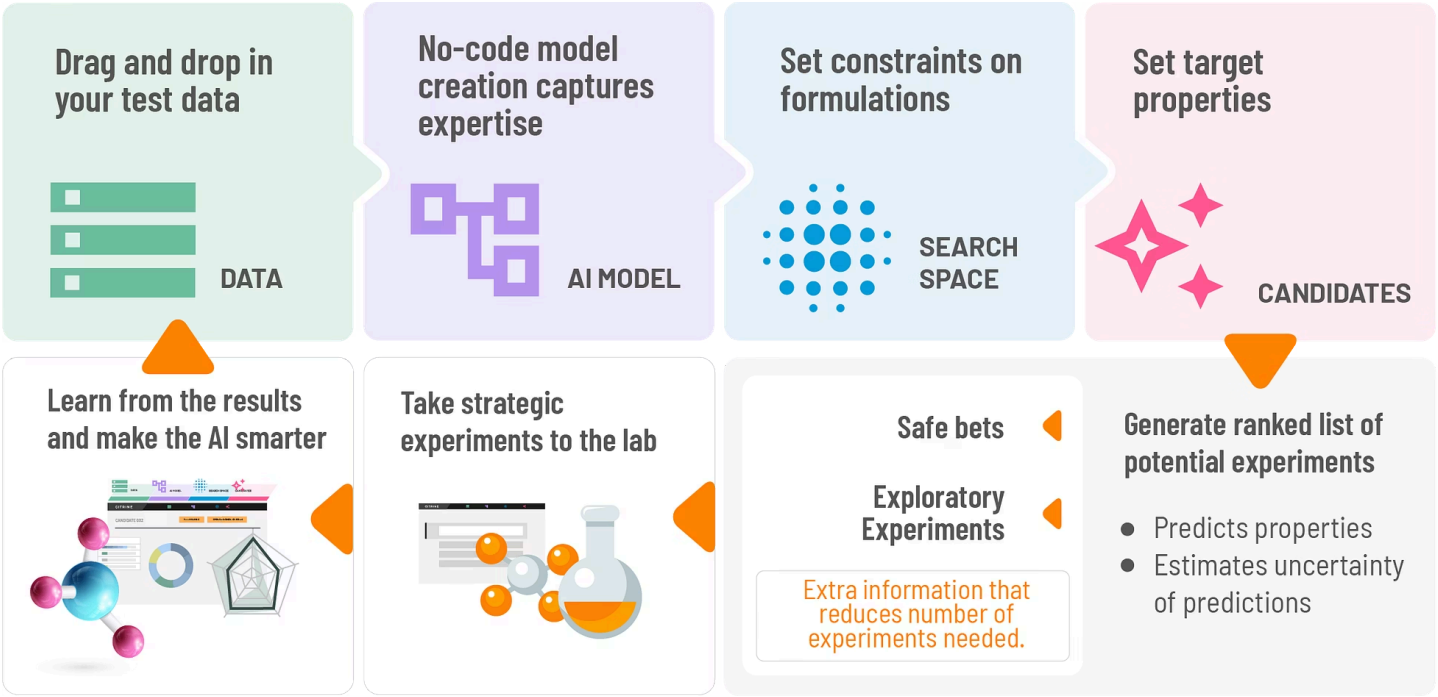
DOE VS. AI-GUIDED EXPERIMENTATION

Choose the experimental method that fits your product development problem

Classical Design of Experiments remains a valuable method for small, stable, well-defined design spaces. Product development gets harder when the variables multiply, conditions shift, and historical data becomes relevant.

AI-guided experimental cycles use predictions and uncertainty to help scientists choose the next experiments, learn from results, and refine the search with each laboratory round.

HOW AI-GUIDED EXPERIMENTAL CYCLES WORK



1. Use initial experimental, simulation, or historical data to build a first model.
2. Define the performance targets, formulation constraints, and scientific boundaries that matter.
3. Compare candidate experiments by predicted performance, probability of reaching the target, and estimated uncertainty. This helps scientists choose between reliable candidates and experiments that could generate the most useful new learning.
4. Scientists choose the next batch based on technical judgment and program priorities.
5. New results improve the model and guide the next experimental cycle.

WHICH APPROACH FITS YOUR WORK?

Criterion	Classical statistical DOE	AI-guided experimental cycles
Minimum data to start	2^n experiments for a full factorial design, where n is the number of variables	Approximately 10–20 initial data points can be practical
Design space	Fully specified at the outset	Iteratively refined with each cycle
Inter-run data pooling	Difficult when response baselines shift over time	Can incorporate heterogeneous data with uncertainty-calibrated modeling
Number of variables	Practical limits often emerge around 6-8 variables	Can accommodate many variables, including molecular descriptors
Model transparency	Regression coefficients, R^2, residual plots	Feature importance, impact plots, prediction and uncertainty outputs
Boundary experiments	Often needed to define the design space	Constraints can be applied directly
Missing data	Can weaken a fixed design	Accommodated through increased local uncertainty
Best use	Small, stable, well-defined problems	Complex, evolving, multi-variable product development

BEGIN WITH THE DECISION YOUR TEAM NEEDS TO MAKE

DOE and AI-guided experimentation are complementary tools. Use DOE when the problem is compact and stable. Consider AI-guided experimental cycles when a team needs to learn across a large, changing design space and make each laboratory round more informative.

Ready to discuss a product development challenge?

Request a Meeting

CITRINE INFORMATICS