

How to Choose AI Software for Product Development



Many organizations have strategic goals to digitalize innovation. With so many options out there, it is hard to decide which organization to partner with. This flow chart aims to give you hints on what to think about as you make the decision.

Are your projects simple, with fewer than 5 raw materials and processing parameters to consider?

Yes → You could use DOE

JMP and Minitab are options

DOE is great for simple projects with few variables to optimize. However, the number of experiments needed can scale exponentially with the number of variables AI is more efficient for more complex projects.

No

Are you doing a one off project?

Yes → Consider partnering with a local university or consultant

This can be cost effective as long as you do not plan to do many projects, or want to use AI in the company's day-to-day workflow.

No

Do you have an in-house team of software engineers and data scientists?

Yes → You could build your own system

- Check how long it will take them to build the system, as this may significantly delay time to value.
- Make sure that they can produce secure, easy-to-use, scalable, enterprise software.
- Have a plan for how to keep it up-to-date and cutting-edge.

No

Do you have large datasets with hundreds of thousands of data points?

Yes → You could use generic AI systems built for "Big Data"

IBM Watson, DataRobot, Amazon Sage Maker... are options

These systems were built to exploit large datasets regardless of the industry you are in.

No

Are lab workflows and data management for regulatory compliance your primary concern, with AI as a nice to have?

Yes → You could use an ELN or LIMS system

Alchemy, Biovia, Uncountable, Benchling are options

These systems were built to manage and route data around a lab. They have lately tried to add AI capabilities.

No

Use an AI platform built for materials, chemicals or product innovation.

Citrine Informatics, Noble AI, Intellegens are options

Things to look for:

- Chemically-aware - interprets molecular structure, chemical formulas etc.
- Understands formulations and can optimize with complex constraints
- Able to featurize new ingredients and predict how they will affect a product
- Flexible but robust data model, able to easily accept new data sources
- An attractive and intuitive user interface that allows product developers to build and leverage AI models to development products with only a few hours training
- Sophisticated uncertainty quantification to cope with small datasets
- Automatically creates default AI models - empowering product experts to use AI
- Captures the knowledge of your experts and uses it to accelerate innovation
- An experienced support team with experts in chemistry, materials science, AI, and change management