NOBLEAI

Solution Brief: NobleAI Model Builder

Build and Train Science-Based AI Models Without Code

Challenge: Accelerating AI Model Development in Scientific R&D

Building custom AI models for scientific applications is traditionally slow, resource-intensive, and dependent on specialized data science expertise. Scientists and product developers face barriers that slow discovery and increase R&D costs:

- Long model development cycles delay innovation and time-to-market
- Limited access to AI expertise hinders experimentation and iteration
- Difficulty integrating scientific knowledge into general-purpose AI tools
- Poor model interpretability reduces confidence in predictions
- Fragmented or inefficient workflows limit collaboration and reuse across teams

When bottlenecks compound, even established organizations struggle to turn ideas into outcomes. Product, R&D, and business teams spend more time managing data and queued model workflows than testing scenarios or refining formulations, which slows innovation, raises costs, and misses windows in fast-moving markets.

Solution Overview: Democratizing Science-Based AI Model Creation

NobleAI's Science-Based AI (SBAI) Model Builder empowers scientists, formulators, and product developers to build and apply custom AI models tailored to their unique R&D challenges—without writing a single line of code.

Built on NobleAI's Visualizations, Insights & Predictions (VIP) Platform, Model Builder combines proprietary science-based algorithms with intuitive design and automated optimization. Users can select between generic and formulation-specific model types, configure datasets, and define input and output parameters. The platform automatically evaluates multiple algorithm and featurizer

combinations to generate interpretable, high-performing models that can be deployed directly within R&D workflows.

Key Capabilities:

- **No-code model creation:** Intuitive workflow to build & train models using your own data.
- **Formulation-specific and generic models:** Choose the right model type for materials formulation or general scientific tasks.
- **Automated optimization:** Platform evaluates multiple algorithms and feature combinations to identify top-performing models.
- **Interpretable AI:** Built-in metrics and visualization tools provide transparency into model performance and prediction rationale.
- **Seamless deployment:** Deploy models directly within the VIP Platform for prediction, analysis, and workflow integration.

The result: faster, more confident decision-making through science-based, interpretable AI that transforms experimental data into actionable insight.

How It Works

1. **Select Model Type** – Choose between a generic or formulation-specific model.
2. **Upload Data** – Import datasets (CSV, Excel) and assign parameters as inputs or outputs.
3. **Configure Training** – Define the train-test split and evaluation metrics (R^2, RMSE, MSE, MAE).
4. **Optimize Automatically** – Model Builder runs multiple algorithms (Random Forest, Gradient Boosting, Neural Networks) to find the best performer.
5. **Review and Select** – Compare ranked models and performance metrics, then deploy the best model for real-time predictions.
6. **Deploy and Use** – Apply the deployed model within R&D workflows to explore results, test hypotheses, and accelerate development.

Key Benefits & Use Cases

- **Accelerate R&D cycles and discovery:** Reduce model development time from months to minutes.
- **Democratize AI adoption:** Empower scientists and engineers to build and apply AI directly, scaling innovation without additional resources.
- **Predict performance and outcomes:** Use formulation data to identify high-potential candidates faster.

- **Enhance collaboration:** Shared dashboards and model insights align teams across research and product functions.
- **Increase sustainability and efficiency:** Identify optimal solutions earlier, reducing costly experimentation and waste.

Technical Highlights

Attribute	Description
Product Name	Model Builder
Supported Model Types	Generic, Formulation
Target Users	Scientists, formulators, and product developers in chemistry, materials science, and energy
Data Input	CSV or Excel files with defined input/output parameters
Optimization	Automated algorithm and featurizer selection
Evaluation Metrics	R^2, RMSE, MSE, MAE
Deployment	Cloud-based within VIP Platform
Interpretability	Feature importance, performance metrics, visual diagnostics

About NobleAI

Backed up by Chevron Technology Ventures, Microsoft M12 and several leading venture capital firms, NobleAI delivers practical AI solutions for complex challenges in chemistry and energy. Our data-efficient Science-Based AI (SBAI) technology, combined with the powerful Visualizations, Insights & Predictions (VIP) Platform, enables customers to compress months of R&D work into minutes. Built on secure, enterprise-ready technology and trusted by global leaders, NobleAI helps companies drive innovation, reduce costs, and accelerate sustainability goals.

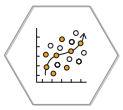
With SBAI on the VIP Platform, teams can quickly test formulations and eliminate unviable options, democratizing AI and enabling faster, more confident innovation.

VIP (Visualizations, Insights & Predictions) Platform

Deploy Your Own Models (DYOM)
Run your existing models to accelerate insights, reduce bottlenecks, and enable collaboration.

Model Builder for Formulations (MBFF)
Build and train your own SBAI models. No coding or data science expertise needed.

Inverse Designs With Parameter Sweeps
Identify the optimal results based on multiple, predefined goals and constraints.

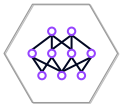


Forward Prediction With Parameter Sweeps
Generate formulation predictions and run unlimited experiments in software with parameter sweeps.

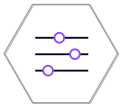
Dynamic Visualization
Visualize and analyze data using customizable data, graphs, and tables.

Deep Insights
Understand predictions through uncertainty, confidence, probability, and feature impacts.

Science-Based AI Models



Ensemble Model Architecture
SBAI Models are built from multiple individually trained model elements.



Customized Solution
SBAI models are structured, created and optimized for each specific use case.

Multi-Science, Multi-Scale
SBAI can incorporate any physical law, chemical property, scientific principle or constraint.

Data Efficiency and Privacy
SBAI models don't need to learn scientific principles from data and are inherently private.