



The Role of AI in Tomorrow's Laboratories

Presented by Ian Fletcher | Enterprise Account Executive | Uncountable

Uncountable

About Uncountable



Originally Founded in 2016

• Offices:

- San Francisco, CA (HQ)
- New York City, NY
- Munich, Germany



100+ Customers Across Industries

• Enterprise R&D Teams:

- Paints & Coatings
- Cosmetics
- Advanced Materials
- Food & Beverage
- Pharma & BioTech
- Adhesives
- Agriculture



#1 End-to-End R&D Platform

• One Source of Truth:

- Centralized data management, capture, & access across all teams
- Reduces new product dev. timelines & iterations
- Predictive analytics & formulation suggestions
- Connected data across systems and databases



Proven Domain Expertise

• Founded by Experts

- Began as a data science company helping Fortune 500 materials companies accelerate development of new projects
- Leveraged learnings to develop a platform focused on structured data to enable proper AI-driven insights



Uncountable Proudly Supports Clients

Across a Variety of Industries



Agenda

- I. **The AI Imperative**
- II. **Business Value: The Formula Market Leaders**
- III. **AI, ML, & LLMs in R&D**
- IV. **Q&A**

Section I. The AI Imperative

AI won't replace scientists.

But scientists who use AI will replace those who don't.

The AI Imperative

- **The Need to Innovate The Process of Innovating**

- R&D is undergoing a major transformation: From trial-and-error to data-driven design
- AI enables faster innovation cycles, deeper insights, and cost savings.

- **R&D faces challenges across segments worldwide**

- Global Competition
- Regulatory & Compliance Complexity
- Sustainability Mandates & Ingredient Sourcing
- Data Silos & Poor Data Infrastructure
- Complex Consumer & Market Demands

- **David Baker, Demis Hassabis and John Jumper awarded with the Nobel prize for Chemistry 2024 for their *protein folding model* from Google's Deepmind project**

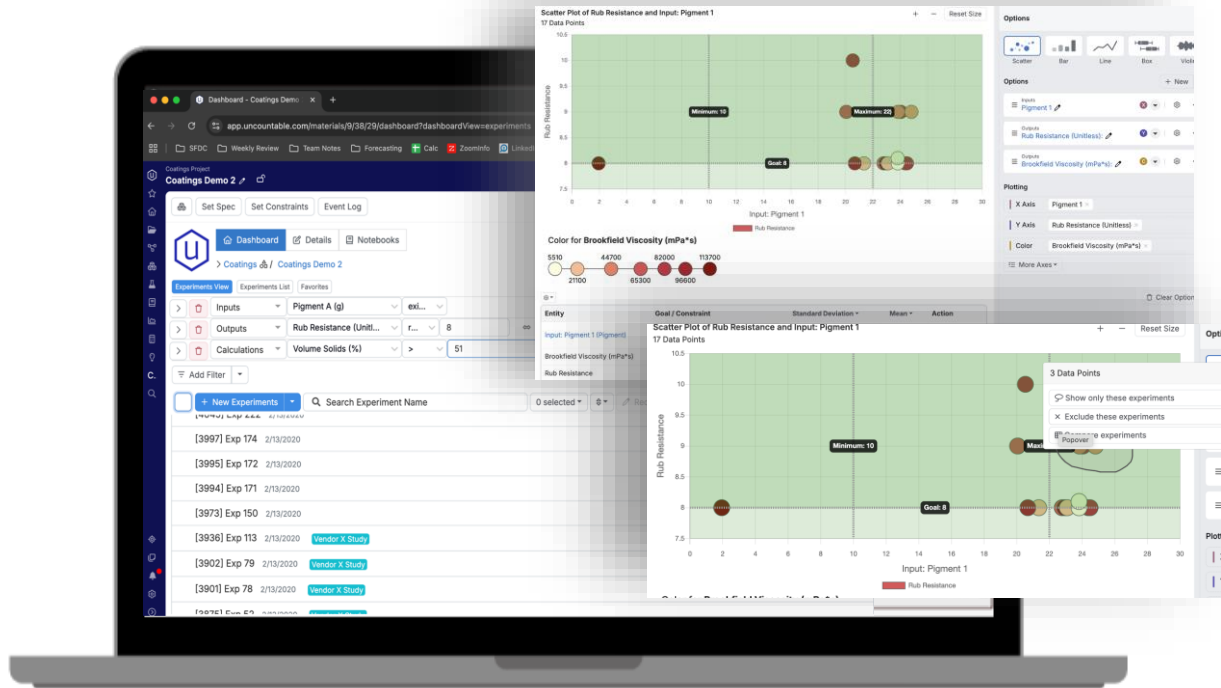
- Growing importance of AI in advancing scientific discovery and addressing complex challenges
- Demonstrates significant advancement and prevalence of AI and how much more potential there is to explore



The Future of Digital R&D = Structured & Actionable Data

Uncountable makes it easy for scientists to **search, filter, and track experiments across projects**, while seamlessly **capturing interconnected data at every stage and every step of your R&D lab's processes**.

Leverage all your **rich, clean, and structured data** to automatically fuel **Uncountable's proprietary scientific AI & ML models**—allowing your organization to **uncover insights and drive continuous improvements faster and faster** with every new data point that's captured.

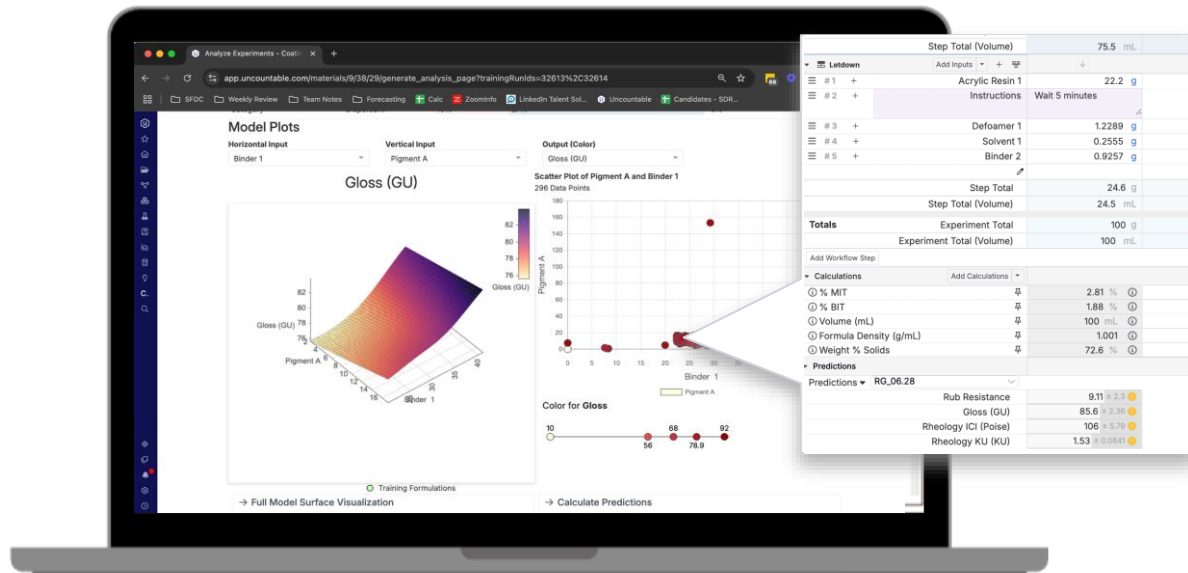


The Future of Digital R&D = AI-Enabled

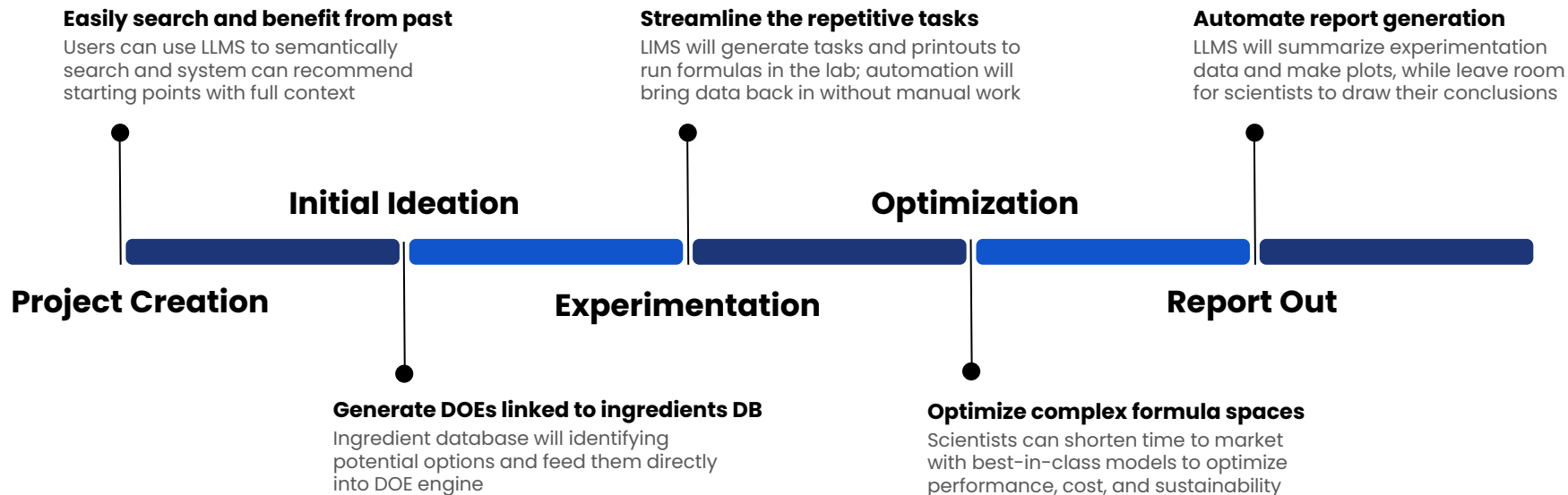
Maximize insights from *all* experiments—successes and failures—using AI to facilitate **fully data-drive decisions**.

Optimize resource use and accelerate innovation cycles by over 50% with AI-enabled formulation and DoE strategies.

Leverage Uncountable's unified R&D data repository to speed up product development and **accelerate go-to-market timelines**.



Utilizing AI to Automate & Augment Scientists



Section II. Business Value

*The question isn't **whether AI can have an impact.***

*It's whether companies are implementing AI for
use cases **with the potential to drive business value.***

Expected Impacts of AI Surveyed

- **According to a 2024 McKinsey & Company survey of R&D leaders, expected impacts include*:**
 - **20% to 50% increase in product-market fit**
 - Integrating AI to expand and explore the solution space of design concepts and uncover how inputs affect outputs—driving deeper understanding and faster innovation in your formulations.
 - AI Analytics
 - Raw Material Replacement
 - **15% to 60% increase in product performance**
 - Leveraging deep-learning surrogates to evaluate performance, see predictions, and receive explanations to help make informed adjustments to formulations before using valuable resources on lab samples
 - Predicting Performance
 - **30% to 50% increase in workplace productivity**
 - Using a virtual lab assistant to input freeform text requests to easily search or visualize data and receives structured filters and plots in return.
 - Voice-to-Text / Text-to-Voice
 - **20% to 40% reduction in time-to-market**
 - ML-driven DOEs are iterative, adapting with each new data point to continuously refine models to deliver results with 30% - 40% fewer experiments compared to traditional methods.
 - Suggesting Experiments

*(Source: McKinsey & Company. (2024, March 26). Using AI to supercharge R&D: Takeaways from the R&D Leaders Forum.)



Leveraging AI in R&D: Achieving a Competitive Advantage

Future Prospects & Trends in AI-Driven R&D

- From Assistive to Autonomous R&D
- Foundation Models & LLMs in Scientific Workflows
- AI-Augmented Human Expertise
- Scalable Institutional Knowledge Capture & Use
- Ethics, Regulation, and Responsible AI
- Sustainability-Driven Innovation
- AI for Multiscale & Multimodal Science

Ways AI Can Enhance R&D Performance & Competitiveness

- **Short-Term**
 - Accelerated Data Analysis & Pattern Recognition
 - Reduced Time-to-Insight
 - Improved Decision-Making
 - Workflow Automation
 - Cost Savings in Experiments
- **Long-Term**
 - Faster Innovation Cycles
 - Improved Product Success Rates
 - Knowledge Retention & Reuse
 - Competitive Differentiation
 - Scalable Collaboration Across Functions & Sites



Uncountable AI Tools Overview

Tool	Type	Function	Key Benefit
Model Building	ML	Trains models on historical formulation and experimental data	Derives insight from past experiments and relationships
Predictive Performance	ML	Forecasts performance of new formulations before physical testing	Reduces costly and time-consuming lab work
Suggesting Experiments	ML	Recommends high-value next experiments based on current data	Accelerates iteration and maximizes learning per experiment
Raw Material Replacement	LLM	Identifies viable substitutes for raw materials	Ensures supply chain resilience and drives cost/sustainability gains
PDF Parser	LLM	Extracts structured info from technical PDFs	Makes historical and third-party knowledge searchable and usable
Voice-to-Text	LLM	Transcribes voice commands to log results and organize input into structured records.	Streamlines workflows & enables hands-free efficiency.
Text-to-Action	LLM	Input freeform text requests to automate collection and generation of information	Easily search or visualize data and receives structured filters and plots in return.



How ML & LLMs Differ & Complement in R&D

Machine learning accelerates what we do in the lab, while large language models unlock why we did it and what we already know — together, they compress the R&D timeline and make innovation more repeatable

AI in R&D		
Category	ML in R&D	LLMs in R&D
Data Type	Learns from structured experimental data	Learns from both structured & unstructured text
Key Function	Optimizes formulations and process parameters	Surfaces relevant knowledge and context
Use Cases	Predicts results and recommends new formulas	Explains results, suggests hypotheses



Section III. AI & Machine Learning in

R&D

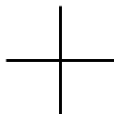
*Understanding that ML models **require large amounts of data** to train from is **critical** if you expect it to return **accurate results**.*

Uncountable began as a **data science company** that provided services to **Fortune 500 materials companies** to **help accelerate the development of new projects**.



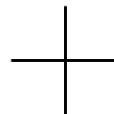
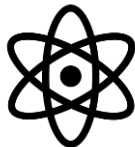
Jason Hirshman
CTO & Co-Founder

Stanford A.I., Palantir, and StartX. Studied Math & CS at Stanford.



Noel Hollingsworth
CEO & Co-Founder

Second Spectrum and Forbes 30 under 30. Studied CS at MIT.



Will Tashman
CRO & Co-Founder

Product Designer at Apple. Studied Materials Science at MIT.



How AI Powers The R&D Lifecycle

PHASE	AI CAPABILITIES
Idea Generation	Literature review, patent mining (LLMs)
Experiment Design	Recommending next best experiments (ML)
Data Collection	Auto-capturing lab notes, digitizing observations (LLMs)
Analysis	Pattern detection, multivariate regression (ML)
Knowledge Management	Semantic search across documents, automated reports (LLMs)
Decision Support	Synthesizing insights for go/no-go decisions



Where LLMs Help vs. Don't Help

High-Impact Use Cases

- **Knowledge Retrieval**
 - Semantic search across ELNs, lab reports, patents, and publications
- **Experiment Documentation**
 - Auto-summarizing methods, outcomes, and hypotheses
- **Cross-Functional Communication**
 - Translating technical results into plain English for execs or regulatory teams
- **Ideation Support**
 - Suggesting experiment directions based on historical data or literature
- **Training & Onboarding**
 - Answering questions like “Have we tested X before?” or “What does this method mean?”
- **Data Labeling & Categorization:**
 - Tagging unstructured inputs with metadata (e.g., material types, experiment goals)

Limitations: Where LLMs Fall Short

- **Numerical Predictions**
 - LLMs don't calculate precise values from data (ML or physics-based models are better)
- **Data-Driven Modeling**
 - Can't replace ML in regression, classification, or optimization tasks
- **Experiment Design**
 - Not statistically grounded — can't design DOE or optimize experimental matrices
- **Interpretability/Traceability**
 - LLM outputs can be hard to audit or justify in regulated environments
- **Real-Time Applications**
 - Too slow or vague for tight control loops (e.g., in manufacturing)



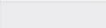
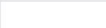
LLM: Ingredient Research

"I'm looking for alternatives to the ingredient Kronos 2220 to help with chalking performance. "

 KRONOS® 2220 is a rutile titanium dioxide (TiO₂) pigment produced via the chloride process. It is specifically designed for plastics applications requiring high outdoor durability and excellent optical properties. The pigment is surface-treated with aluminum, silicon, and polysiloxane compounds, enhancing its performance in various applications.

Key Properties:

- **High Durability:** Enhances the longevity of plastics exposed to outdoor conditions.
- **Brightness and Neutral Tone:** Provides very high brightness with a neutral undertone.
- **Tinting Strength and Opacity:** Offers high tinting strength and opacity, contributing to effective coverage.
- **Dispersibility:** Readily wetted and dispersed, facilitating ease of use in formulations.

	Name	Description	Chemical Info
	Kronos 2190	A rutile titanium dioxide pigment with enhanced weather resistance and surface treatment, designed for outdoor applications with improved chalking resistance.	 Name TITANIUM DIOXIDE Molecular Weight 79.865 g/mol CAS Number 13463-67-7 SMILES O=[Ti]=O
	Tronox CR-828	A chloride-process rutile titanium dioxide pigment with high durability and excellent resistance to chalking, suitable for exterior plastics and coatings.	 Name TITANIUM DIOXIDE Molecular Weight 79.865 g/mol CAS Number 13463-67-7 SMILES O=[Ti]=O



Defining

Unstructured vs. Structured Data:

	Unstructured	vs.	Structured
Examples	• Spreadsheets • Word Documents • PDFs • Lab Journals/ELNs • Shared Drive		• Databases • LIMS • Inventory Systems • Uncountable
Advantages	• Free • Unrestricted entry of information • Known/second nature "habitual"		• Instant access to specific information/data • Shareable & scalable information • Intelligent insights & reporting
Disadvantages	• Limited scope & scalability for application of info • Ctrl+F keyword searching • Limited collaboration • Inability to innovate efficiently & at market-rate		• Requires intentional/deliberate entry of information • Change management • Migration of historical data into new system • Disciplined use



DOEs – Traditional vs. Uncountable

Traditional Methods	Purpose	Uncountable
Parametric regressions, not suited for high dimensional problems	Modeling	Gaussian Processes – Machine learning technique for non-linear, high dimensional spaces
Factorial or partial-factorial suggestions with few variables changing in a rigid and orthogonal search of ingredient space	Experiment Design	Bayesian optimization suggests experiments with best predicted performance and greatest learnings
DOEs are static and independent of previous experiments	Improvement	Machine learning model learns from previous data, improves with each new data point



Repsol: Unlocking Value of Historical Data to Optimize Formulations



- **Customer Since:** 2022
- **Industry:** Energy
- **About Repsol:**

Repsol is a global multi-energy company based in Spain, operating across the entire energy value chain. With a strong focus on innovation and sustainability, Repsol is strongly committed to achieving net-zero emissions by 2050.

Repsol's Advanced Mathematics team used Uncountable to back-test historical and current formulation projects.

The trials showed consistent **savings of 30–40% in formulations per project** compared to prior methods..

Uncountable's native predictive tools ***“allowed [us] to unleash the value of [our] historical data and optimize in silico formulation composition by suggesting to implement, in [our] labs, only those which have better chances to fulfill the product specifications required.”***



Thank You

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