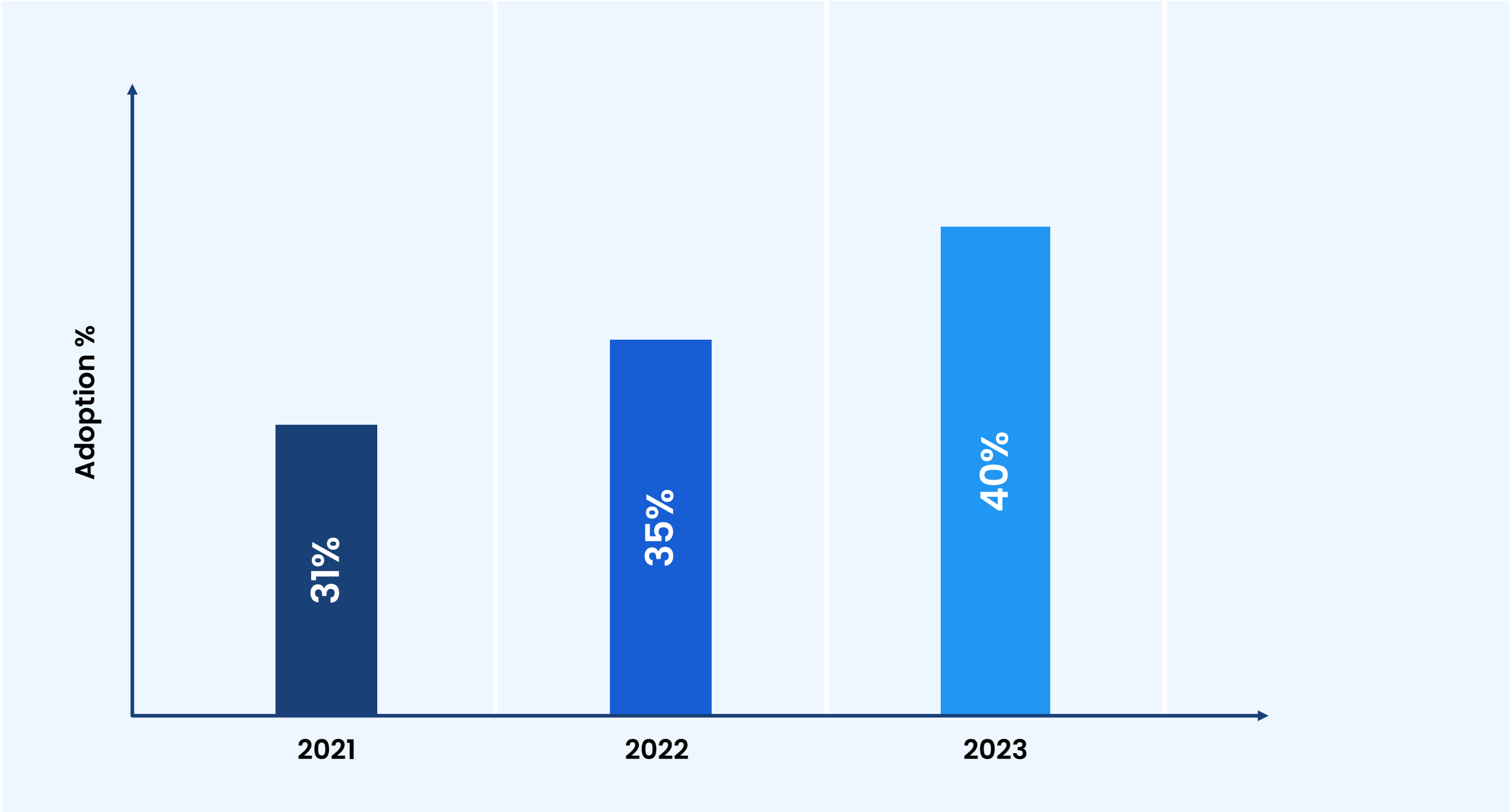# Agenda

- **AI is here!**

- The factors that have historically made it hard to actualize

- How best to overcome these challenges in your organization and achieve positive outcomes with AI

- How to set an actionable AI strategy

Garter has AI at the peak of their hype cycle.

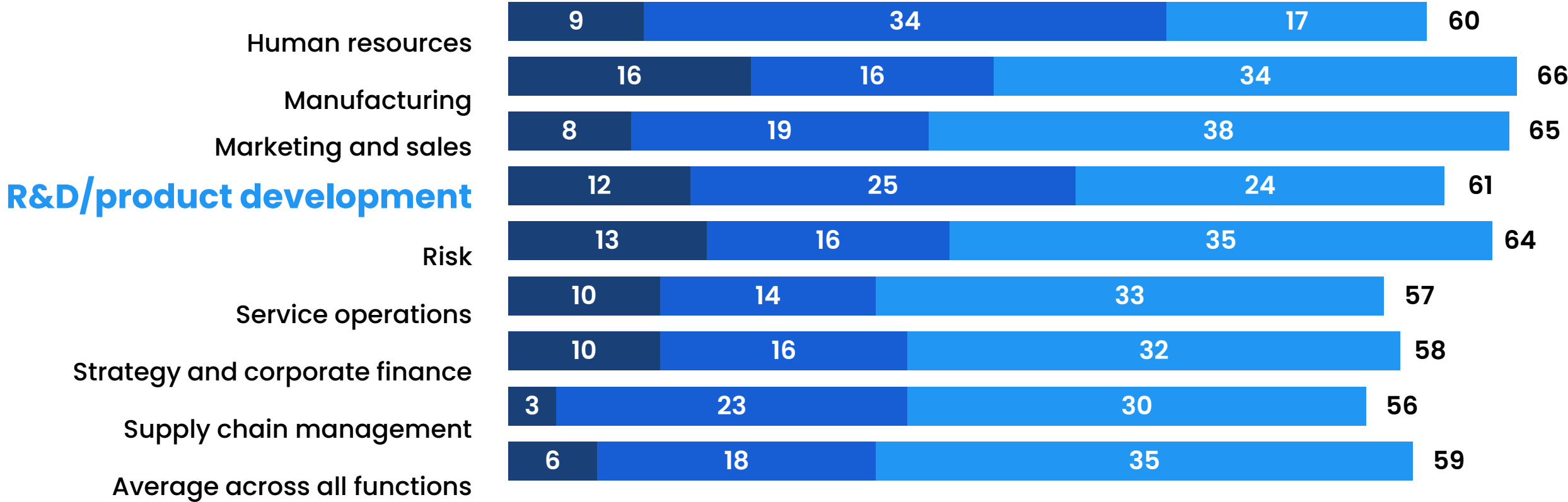**Gartner Hype Cycle for Emerging Technologies, 2023**

Expectations (y-axis) vs Time (x-axis)

Generative AI

- API-Centric SaaS
- Open-Source Program Office
- Cloud-Out to Edge
- **AI TRiSM**
- WebAssembly (Wasm)
- **Federated Machine Learning**
- Industry Cloud Platforms
- Internal Developer Portal
- Cloud Sustainability
- Homomorphics Encryption
- Value Stream Management Platforms
- **Reinforcement Learning**
- Cloud Development Environments
- Graph Data Science
- **AI Simulation**
- **Casual AI**
- Postquantum Cryptography
- **Neuro-Symbolic AI**
- Augmented FinOps
- GitOps
- **Generative Cybersecurity AI**
- Cybersecurity Mesh Architecture

Cloud Native

AI-Augmented Software Engineering

Phases: Innovation Trigger | Peak of Inflated Expectations | Trough of Disillusionment | Slope of Enlightenment | Plateau of Productivity

Time

Plateau will be reached: ○ Less than 2 years ● 2 to 5 years ● 5 to 10 years ▲ 5 to 10 years

AI adoption is steadily growing across all sectors of the economy.

Adoption %

31% — 2021

35% — 2022

40% — 2023

Sources: IBM Global AI Adoption Index 2022; McKinsey State of AI in 2023

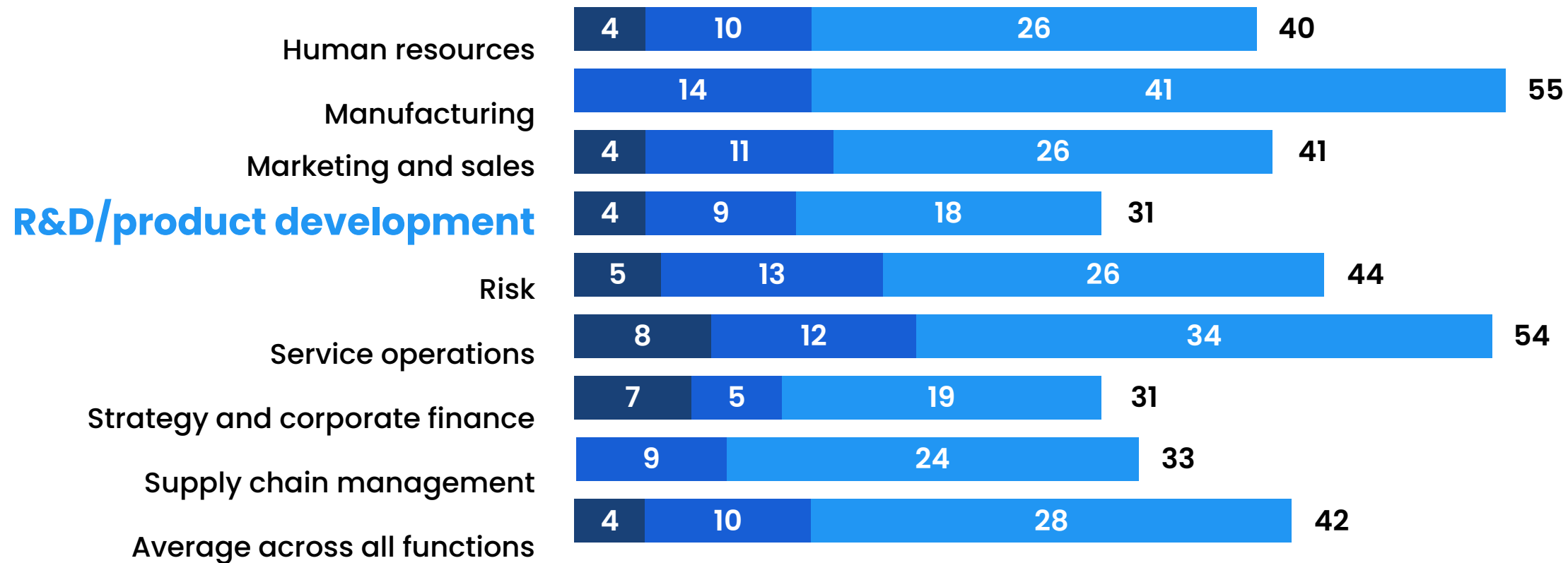# McKinsey data shows meaningful revenue increases from AI adoption.

Revenue increases from AI adoption in 2022, % of respondents

| | >10% | 6-10% | ≤5% |

Human resources — 9 | 34 | 17 — 60
Manufacturing — 16 | 16 | 34 — 66
Marketing and sales — 8 | 19 | 38 — 65
R&D/product development — 12 | 25 | 24 — 61
Risk — 13 | 16 | 35 — 64
Service operations — 10 | 14 | 33 — 57
Strategy and corporate finance — 10 | 16 | 32 — 58
Supply chain management — 3 | 23 | 30 — 56
Average across all functions — 6 | 18 | 35 — 59

As well as cost reductions.

Cost decreases from AI adoption in 2022, % of respondents

Function	≥20%	10-19%	<10%	Total
Human resources	4	10	26	40
Manufacturing		14	41	55
Marketing and sales	4	11	26	41
R&D/product development	4	9	18	31
Risk	5	13	26	44
Service operations	8	12	34	54
Strategy and corporate finance	7	5	19	31
Supply chain management		9	24	33
Average across all functions	4	10	28	42

Source: McKinsey, The State of AI in 2023
n=1,684
https://www.mckinsey.com/capabilities/quantumblack/our-insights/the-state-of-ai-in-2023-generative-ais-breakout-year

And AI "high performers"[1] are driven by upside more than by cost reduction.

Note near **2x** **response rate**

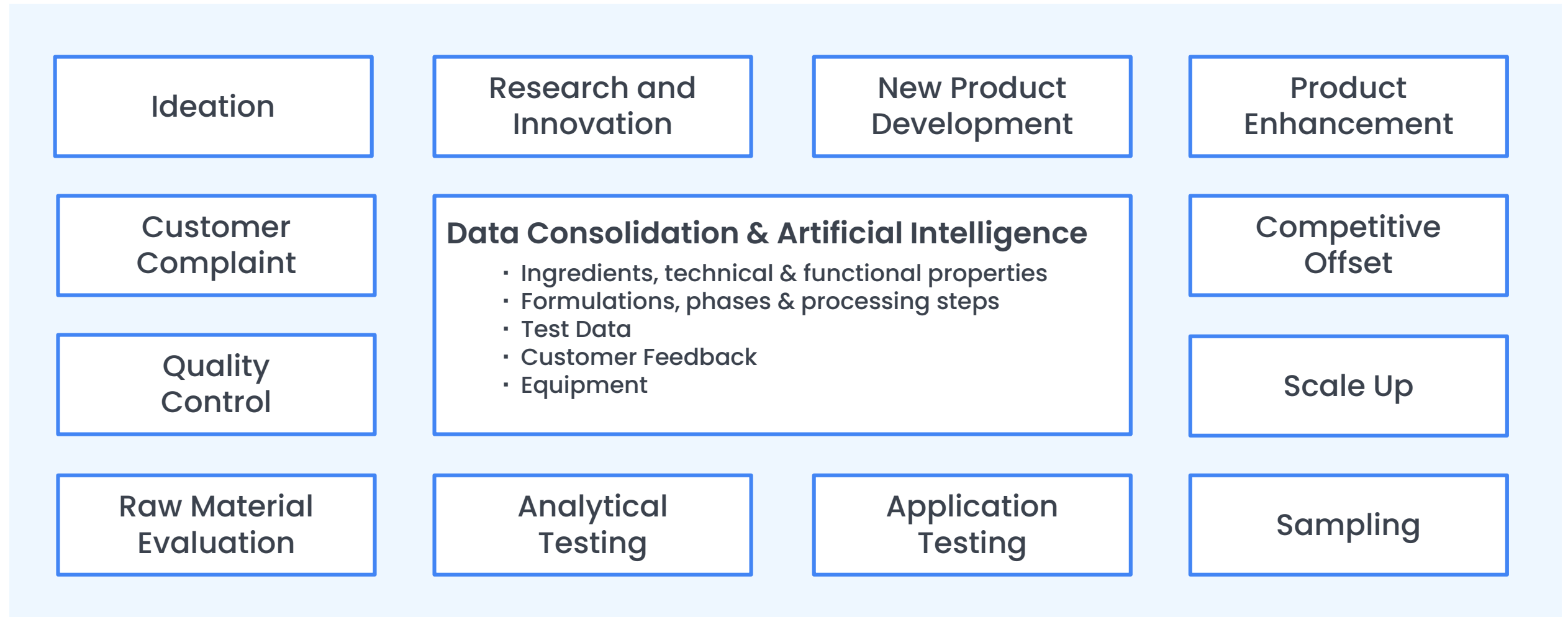|	Respondents at AI **high performers**	All other respondents
Reduce costs in core business	19	33
Create new businesses and/or sources of revenue	23	12
Increase revenue from core business	27	21
Increase value of offerings by integrating AI-based features or insights	30	33

50%

33%

But in practice…

- **80%** of the time spent on AI projects has to do with data curation
  - Find data
  - Determine its relevance
  - Clean data
  - Augment data

- Most companies simply do not have enough AI-ready data to run AI

Agenda

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Each category of work is executed by different teams with different tools in different locations and time zones.
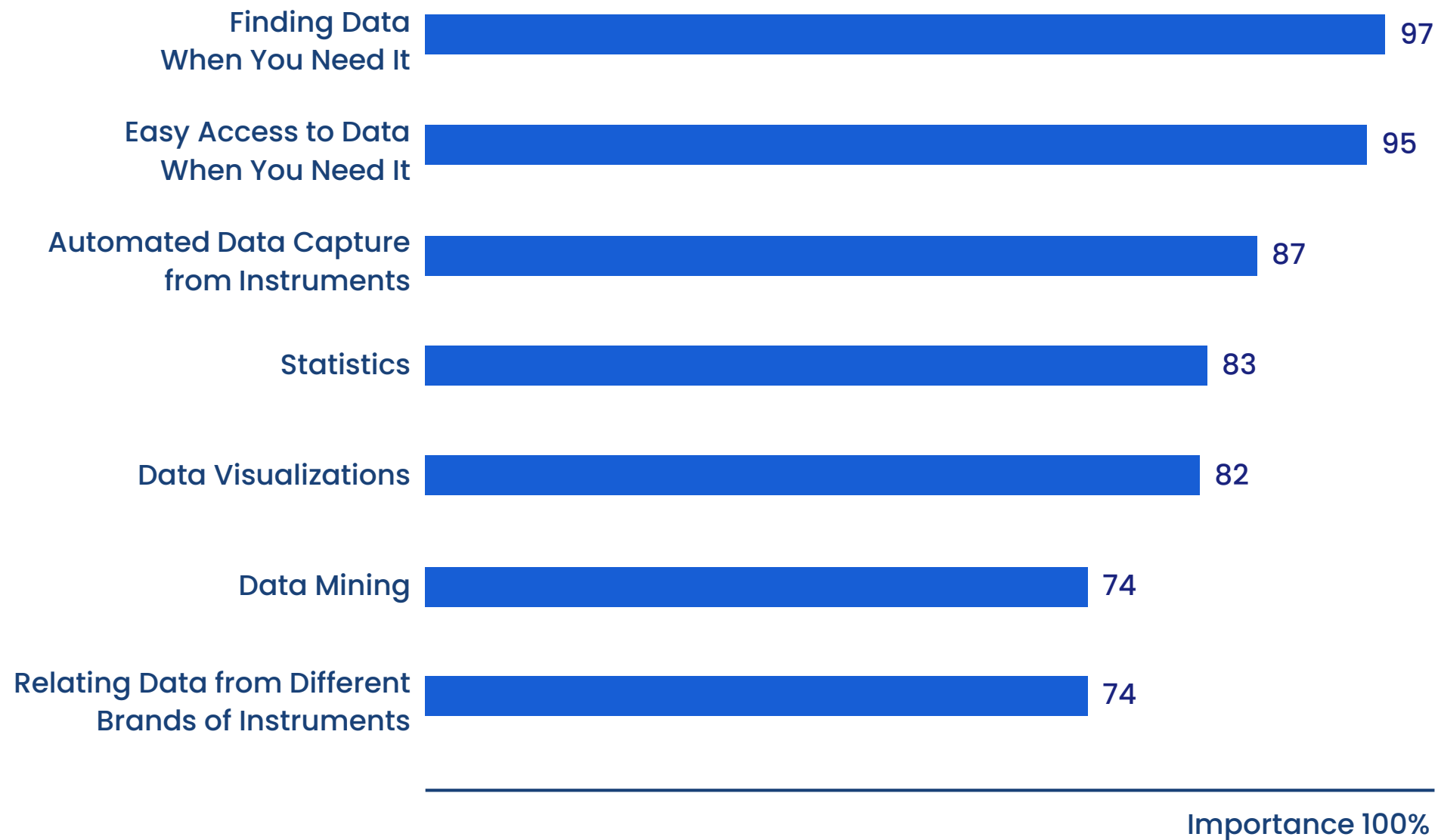
Ideation	Research and Innovation	New Product Development	Product Enhancement

Customer Complaint	**Data Consolidation & Artificial Intelligence** · Ingredients, technical & functional properties · Formulations, phases & processing steps · Test Data · Customer Feedback · Equipment		Competitive Offset
Quality Control			Scale Up

Raw Material Evaluation	Analytical Testing	Application Testing	Sampling

Critical data sits in silos.

Opportunities	Trial Formulations	Final Formulations	Processing Steps	Ambient Conditions	Test Results	Analyses	Customer Feedback	Commercial Result
CRM	Paper Lab Notebook + XLS	Paper Lab Notebook + XLS	Paper Lab Notebook + XLS	Paper Lab Notebook + XLS	Paper Lab Notebook + XLS	Paper Lab Notebook + XLS	Email	Email CRM
Innovation Mgmt	DOE	DOE	DOE	LIMS	LIMS	LIMS	XLS	XLS
XLS	Formulator Software	Formulator Software	Formulator Software	Lab Equipment	Lab Equipment	Statistical Software	CRM	CRM
Presentations	Electronic Lab Notebook	Electronic Lab Notebook	Electronic Lab Notebook	Often not captured	Analytical software	Email + Meetings	Phone calls	ERP
Source of data resides outside the lab	*Not consistently captured or incomplete*	*Often not connected to all associated test results*	*Not consistently captured or incomplete*	*Most frequently omitted*	*Often missing data for failed trial samples*	*Not consistently executed*	*Not consistently captured*	*Source of data resides outside the lab, often long lag*

→ The more software tools, the greater the data degradation, adding time and cost to development.

Nearly every aspect of recording and analyzing data is important.

	Importance
Finding Data When You Need It	97
Easy Access to Data When You Need It	95
Automated Data Capture from Instruments	87
Statistics	83
Data Visualizations	82
Data Mining	74
Relating Data from Different Brands of Instruments	74

Importance 100%

- Chemical & Engineering News Respondents = 700

Data volume is increasing at a faster rate.

(in zettabytes)
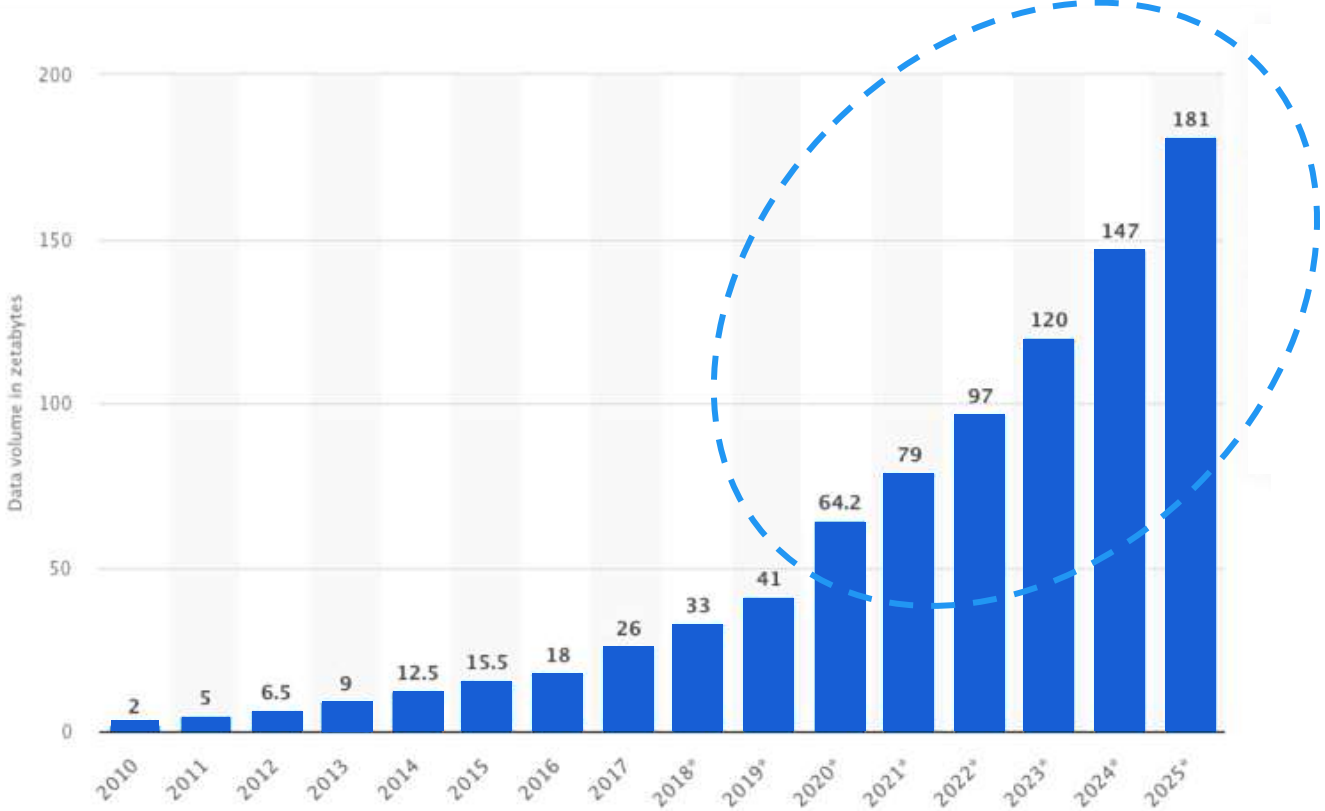
+ By 2025, there will be 75 billion IoT devices, a near 200% increase from today's 26 billion.
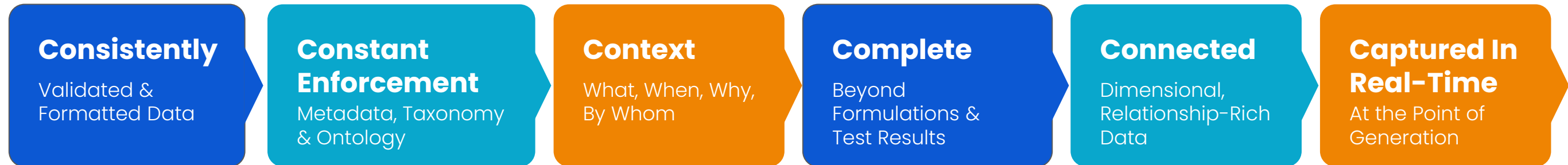
- *Statista, FinancesOnline, Visual Capitalist*

Rolling out AI requires the intersection of software + science.

- New staff

- New skills

- New processes

- New software

- New management metrics

Agenda

1. AI is here

2. The factors that have historically made it hard to actualize

3. **How best to overcome these challenges in your organization and achieve positive outcomes with AI**

4. How to set an actionable AI strategy

Ensure that your data is AI-ready.

Consistently	**Constant Enforcement**	**Context**	**Complete**	**Connected**	**Captured In Real-Time**
Validated & Formatted Data	Metadata, Taxonomy & Ontology	What, When, Why, By Whom	Beyond Formulations & Test Results	Dimensional, Relationship-Rich Data	At the Point of Generation

So that it meets FAIR guiding principles for scientific data management

- **F**indable
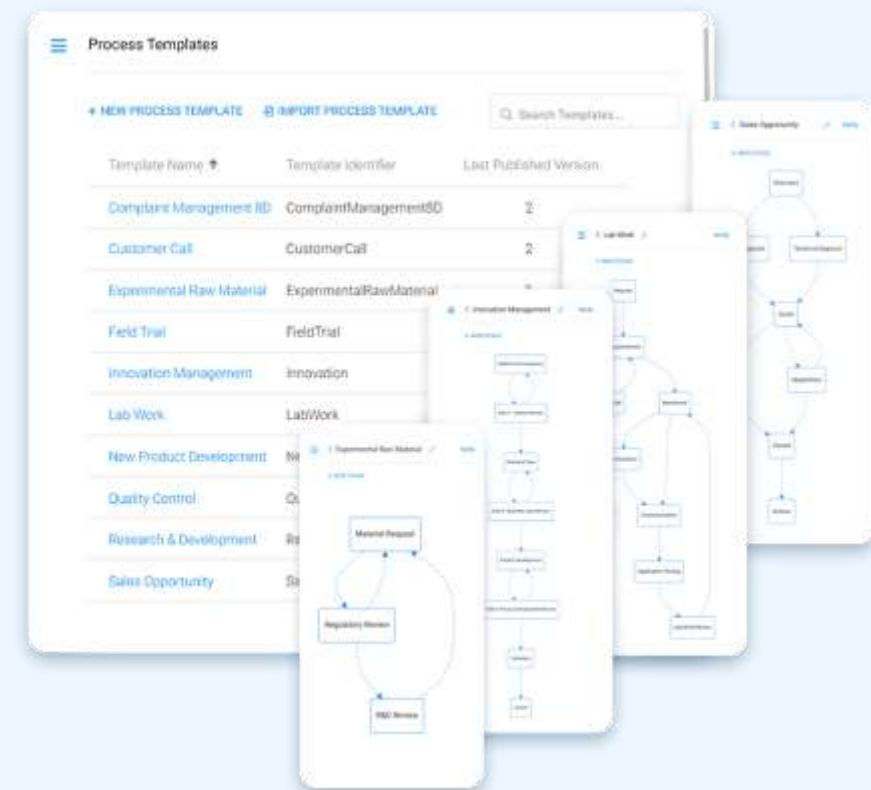- **A**ccessible
- **I**nteroperable
- **R**eusable

Digitizing lab workflows can generate AI-ready data.

No Code Process Automation via Web UI..
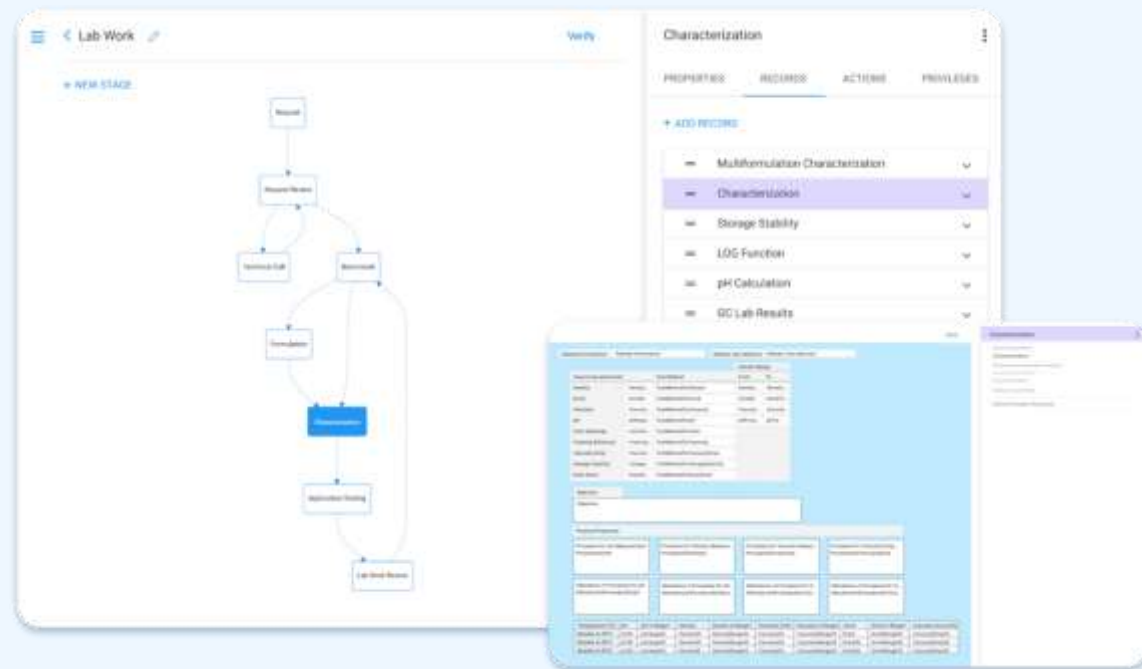
...Generates Custom Lab Applications

Objectives > **Formulations** > **Processing Steps** > **Test Results** > **Insights**
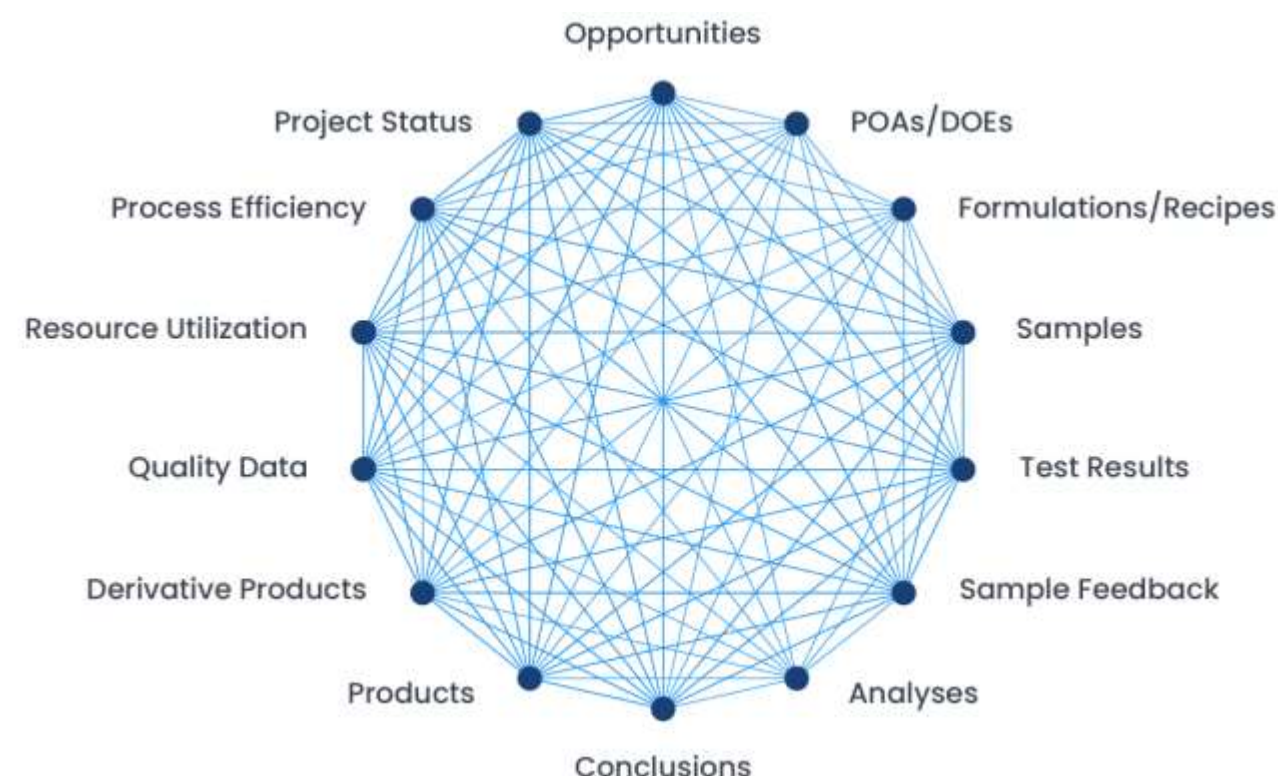
Consolidate technical data in a single source of truth.

Siloed Software & Data

Siloed systems and incomplete, "dirty" data require extensive data prep and have lower predictive value

Unified Data with Embedded AI

Closed-loop systems generate AI-ready data and higher predictive value for chemistry and business use cases

Agenda

1. AI is here

2. The factors that have historically made it hard to actualize

3. How best to overcome these challenges in your organization and achieve positive outcomes with AI

4. **How to set an actionable AI strategy**

AI strategy and objectives.

1. Data curation is the foundation
   - Create, organize and maintain data
   - So it can be accessed and used by people looking for information
   - And make it suitable to train and improve AI models
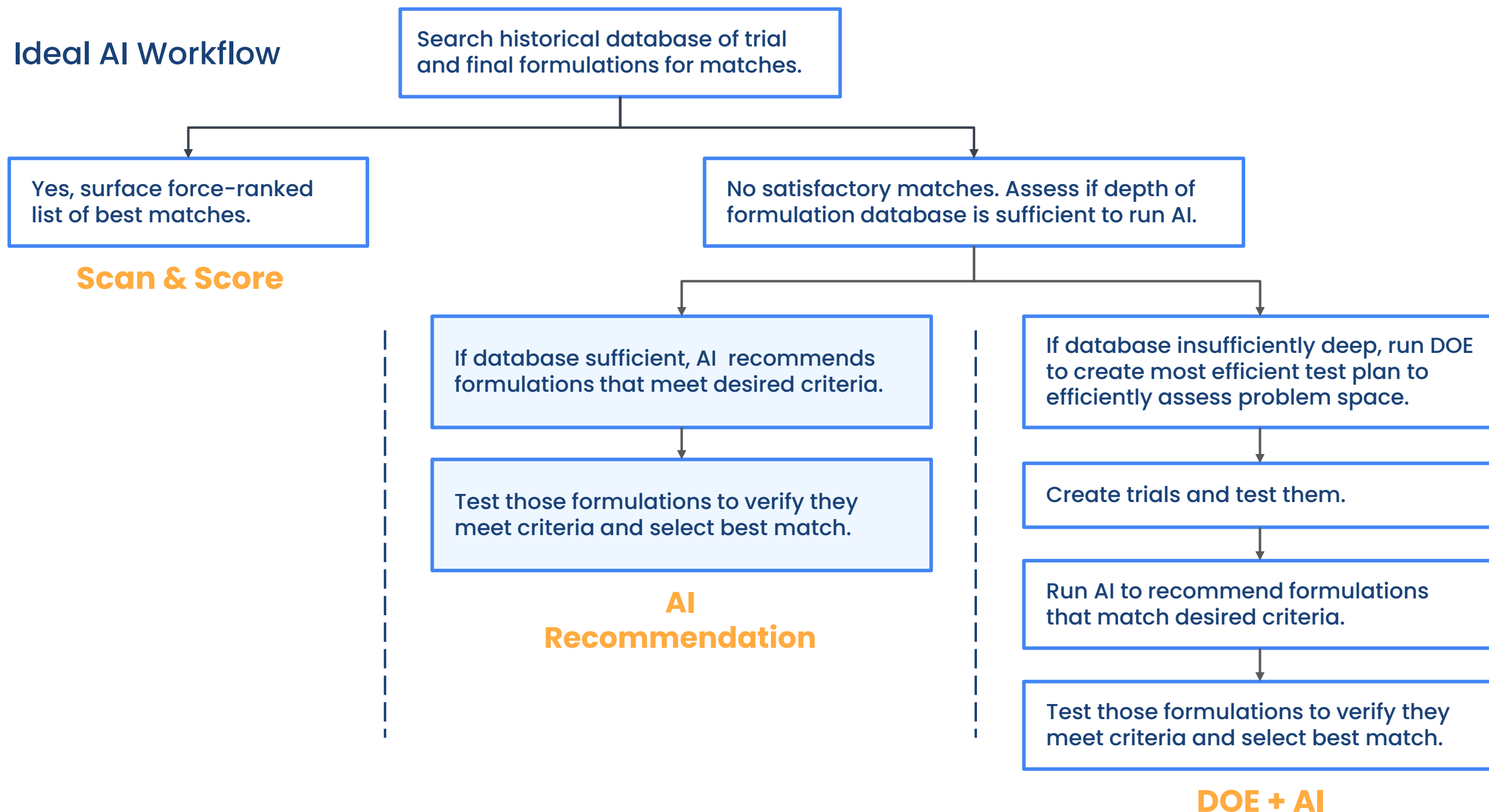
2. Workflow digitalization is the means
   - Digitalizing workflows enables data curation to happen in real-time

3. Data consolidation for AI is a necessary prerequisite
   - This facilitates parameter tuning and model building

4. AI model building in an efficient manner is the **ultimate** objective

Run AI + DOE on the consolidated dataset generated by the software your lab staff uses.

Ideal AI Workflow

Search historical database of trial and final formulations for matches.

Yes, surface force-ranked list of best matches.

Scan & Score

No satisfactory matches. Assess if depth of formulation database is sufficient to run AI.

If database sufficient, AI recommends formulations that meet desired criteria.

Test those formulations to verify they meet criteria and select best match.

AI Recommendation

If database insufficiently deep, run DOE to create most efficient test plan to efficiently assess problem space.

Create trials and test them.

Run AI to recommend formulations that match desired criteria.

Test those formulations to verify they meet criteria and select best match.

DOE + AI

Robust ingredient property data enables both the formulator and AI.

General Information | Hide

Material Name
Novalac Resin, f=3.6

Code
CHAK2189

External Code
43445-12-3

Short Description
Polyfunctional liquid epoxy phenol novolac resin

Procurement
External Material

Standard Cost [$/kg]
13.82

CAS Number
28064-14-4

Material Status
Active

Type
Epoxy Resin

Sub-Type
Novalac

Default Unit
kg

Alternative Units
lb, ton

Alternative Sources | Hide

List of Raw Materials purchased from suppliers

Raw Material	Status	Region	Available Amount [kg]	Cost [$/kg]
EPIKOTE™ Resin 154	Active	Europe	1,850.00	13.82
D.E.R™ 438™	Active	US	560.00	13.50

+ New Raw Material

Material Properties | Hide

Information about physicochemical properties.

Property	Unit	Min	Max
EEW	g/eq.	176.00	181.00

Property	Unit	Min	Max	Temp. [°C]
Viscosity, absolute	cP	31,000	40,000	25.00

Property	Unit	Min	Max
Colour	Pt-Co.	N/A	250

Property	Unit	Min	Max	Temp. [°C]
Density	g/cm³	1.2200	1.2299	25.00

Property	Unit	Min	Max
Hydrolyzable Chloride	ppm	N/A	1,200

Property	Unit	Value
Average Functionality	N/A	3.6

Set your technical and functional targets.

Requirements

Calculations (Calculated properties)

Property	Unit	Priority	Target	
Cost	€/sq.ft.	Nice to have	Lower than	0.484

+ CALCULATION

Tests (Measured properties)

Test method / Property	Unit	Priority	Target	
VOC	%	Must Have	Lower than	6.50
Spray Transfer Efficiency	%	Must Have	Higher than	50.00
Neutral Salt Spray	Hours	Must Have	Higher than	500.00
Ethylene Glycol Immersion - 28...	%	Must Have	Lower than	2.50

+ TEST METHOD   + TEST

Outcome Impacted by Multiple Properties e.g.,

- Viscosity
- Density
- Solids
- Dry Time
- Contact Angle
- Microstructure Coverage
- Dry Film Thickness

Set your formulating constraints.

Material constraints

Materials	Target weight [g]				Mandatory to use
Zinc Phosphate	Between	50.00	-	70.00	Mandatory
EPON 1001-H-75	Between	2.22	-	6.66	Mandatory
DER 438	Between	2.22	-	6.66	Mandatory
Butanol	Constant			6.00	Mandatory
Cellosolve	Constant			5.00	Mandatory
ThixatrolTM ST	Constant			0.30	Mandatory
Surfynol 104 BC	Constant			0.70	Mandatory
EPKURE 3115-E-73	Constant			8.00	Mandatory

+ MATERIAL

Multi-component constraints

Constraints	Materials			Target				
SUM	Zinc Phosphate, EPON 1001-H-75, DER 438			PVC	Higher than			50.00
Ratio	EPKURE 3115-E-73	/	EPON 1001-H-75, DER 438	Weight	Between	0.80	-	1.20

+ CONSTRAINT

[SCAN & SCORE]   [DESIGN EXPERIMENTS]   [PROCEED TO FORMULATING]

Scan & score your historical work.

Formulations

Materials	Material Properties <		S23-001.T01-01	
	Type	Subtype	Weight [%]	Weight [g]
Zinc Phosphate	Pigment	Anti-Corrosion	62.51	50.00
EPON 1001-H-75	Resin	Epoxy BPA	4.16	3.33
DER 438	Resin	Epoxy Novolac	8.33	6.66
Butanol	Solvent	Alcohol	7.50	6.00
Cellosolve	Solvent	Alcohol	6.25	5.00
ThixatrolTM ST	Additive	Rheology	0.38	0.30
Surfynol 104 BC	Additive	Dispersant	0.88	0.70
EPKURE 3115-E-73	Resin	Amine	10.00	8.00
Total			100.00	79.99

Here's the assessment based on your requirements and data base:

Matching formulations
2 Matching Formulations

Predicted targets and confidence intervals

Matching Order			#1		#2	
Formulation Code			S23-001.T01-01		S23-004.T05-03	

Property	Target	Unit	S23-001.T01-01		S23-004.T05-03	
			Value	Confidence	Value	Confidence
Cost	< 0.48	€/sq.ft	0.48	-	0.45	-
VOC	< 6.50	%	1.09	+/- 0.0545	6.37	+/- 0.3185
Spray Transfer Efficiency	> 50.00	%	50.00	+/- 2.5	48.75	+/- 2.4375
Neutral Salt Spray	> 500	Hours	529.00	+/- 26.45	613.00	+/- 30.65
Ethylene Glycol Submersion	< 2.50	%	2.00	+/- 0.1	2.67	+/- 0.1335
Mark for testing			☑		☐	

If no matches, but sufficient pre-existing data, AI can recommend formulations.

Here's the assessment based on your requirements and data base:

Matching formulations
0 Matching formulations

Data for machine learning
Sufficient data for AI   Show detailed analysis

Note: If you want to improve performance of the models choose "Improve the models" to get formulations with the highest uncertainty, otherwise if you are satisfied with performance of the models choose Recommended formulations.

RECOMMEND FORMULATIONS

Materials	Material Properties		ML23-001-01	
	Type	Subtype	Weight [%]	Weight [g]
Zinc Phosphate	Pigment	Anti-Corrosion	63.39	50.00
EPON 1001-H-75	Resin	Epoxy BPA	2.81	2.22
DER 438	Resin	Epoxy Novolac	8.44	6.66
Butanol	Solvent	Alcohol	7.61	6.00
Cellosolve	Solvent	Alcohol	6.34	5.00
ThixatrolTM ST	Additive	Rheology	0.38	0.30
Surfynol 104 BC	Additive	Dispersant	0.89	0.70
EPKURE 3115-E-73	Resin	Amine	10.14	8.00
Total			100.00	78.88

Predicted targets and confidence intervals

Matching Order			#1		#2	
Formulation Code			ML23-001-01		ML23-001-02	
Property	Target	Unit	ML23-001-01		ML23-001-02	
			Value	Confidence	Value	Confidence
Cost	< 0.48	€/sq.ft	0.48	-	0.40	-
VOC	< 6.50	%	1.99	+/- 0.0995	3.20	+/- 0.16
Spray Transfer Efficiency	> 50.00	%	51.00	+/- 2.5	50.00	+/- 2.5
Neutral Salt Spray	> 500	Hours	536.00	+/- 26.8	500.00	+/- 25.00
Ethylene Glycol Submersion	< 2.50	%	1.00	+/- 0.05	2.00	+/- 0.10
Mark for testing			☐		☐	

If there is insufficient data, use DOE to design experiments to learn more, faster.

Here's the assessment based on your requirements and data base:

Matching formulations

0 Matching formulations

Data for machine learning

Insufficient data

Show detailed analysis

DOE - Screening design

8 Formulations needed

Informed by your database findings, we suggest embracing design of experiment for formulating design.

DESIGN EXPERIMENTS

Formulations

Materials	Material Properties <		DOE23-001-01		DOE23-001-02	
	Type	Subtype	Weight [%]	Weight [g]	Weight [%]	Weight [g]
Zinc Phosphate	Pigment	Anti-Corrosion	63.39	50.00	63.39	50.00
EPON 1001-H-75	Resin	Epoxy BPA	8.44	6.66	2.81	2.22
DER 438	Resin	Epoxy Novolac	2.81	2.22	8.44	6.66
Butanol	Solvent	Alcohol	7.61	6.00	7.61	6.00
Cellosolve	Solvent	Alcohol	6.34	5.00	6.34	5.00
ThixatrolTM ST	Additive	Rheology	0.38	0.30	0.38	0.30
Surfynol 104 BC	Additive	Dispersant	0.89	0.70	0.89	0.70
EPKURE 3115-E-73	Resin	Amine	10.14	8.00	10.14	8.00
Total			100.00	78.88	100.00	78.88

Create your formulations, test them, enter the results, and then run AI.

Formulations

Materials	Material Properties ‹		DOE23-001-01		DOE23-001-02		DOE23-001-03		DOE23-001-04	
	Type	Subtype	Weight [%]	Weight [g]	Weight [%]	Weight [g]	Weight [%]	Weight [g]	Weight [%]	Weight
Zinc Phosphate	Pigment	Anti-Corrosion	63.39	50.00	63.39	50.00	64.29	50.00	65.22	
EPON 1001-H-75	Resin	Epoxy BPA	8.44	6.66	2.81	2.22	5.71	4.44	4.34	
DER 438	Resin	Epoxy Novolac	2.81	2.22	8.44	6.66	4.28	3.33	4.34	
Butanol	Solvent	Alcohol	7.61	6.00	7.61	6.00	7.72	6.00	7.83	
Cellosolve	Solvent	Alcohol	6.34	5.00	6.34	5.00	6.43	5.00	6.52	
ThixatrolTM ST	Additive	Rheology	0.38	0.30	0.38	0.30	0.39	0.30	0.39	
Surfynol 104 BC	Additive	Dispersant	0.89	0.70	0.89	0.70	0.90	0.70	0.91	
EPKURE 3115-E-73	Resin	Amine	10.14	8.00	10.14	8.00	10.29	8.00	10.44	
Total			100.00	78.88	100.00	78.88	100.00	77.77	100.00	

Calculations

Property	Target	Unit	DOE23-001-01	DOE23-001-02	DOE23-001-03	DOE23-001-04
			Value	Value	Value	Value
Cost	< 4.84	€/sq.ft.	0.33	0.48	0.37	

Tests

Property	Target	Unit	DOE23-001-01 ›	DOE23-001-02 ›	DOE23-001-03 ›	DOE23-001-04 ›
			Value	Value	Value	Value
VOC	< 6.50	%	4.16	7.32	6.50	
Spray Transfer Efficiency	> 50.00	%	60.00	46.67	51.67	
Neutral Salt Spray	> 500	Hours	465.00	440.00	484.00	
Ethylene Glycol Submersion	< 2.50	%	3.67	1.00	3.25	

TRAIN PREDICTIVE MODELS

With that data, get AI-recommended formulations with predicted properties.

Machine Learning Recommendations

Alchemy has generated 4 formulations that match your targets.

Statistical Result Details Hide

| Properties	Best Performing Model	R² - train	R² - test	Mean Squared Error - train	Mean Squared Error - test
VOC	Linear Regression	0.9997	0.9805	0.00005	0.00044
Cost	Calculation	N/A	N/A	N/A	N/A
Transfer efficiency of spray-applied ...	XGBoost	0.8726	0.8135	1.35633	7.825332
Neutral Salt Spray	Random Forest Reg...	0.8893	0.8762	15.9391	17.64836
10% Acetic acid submersion - 28 days	Random Forest Reg...	0.8326	0.8145	0.097	0.1222

Generated Formulations

| Properties	Unit	ML-1814-001 ‹ Value	In range	Confidence	Best Performing Model	ML-1814-002 › Value	In range	ML-1814-003 › Value	In range	ML-1814-004 › Value	In range
VOC	%	4.50	In range	± 0.20	Linear Regression	4.70	In range	5.00	In range	4.70	In range
Cost	$/sq m	4.69	In range	N/A	Calculation	4.72	In range	4.89	Out of range	5.01	Out of range
Transfer efficiency of spray-applied ...	%	73.20	In range	± 10.20	XGBoost	65.20	In range	71.20	In range	70.50	In range
Neutral Salt Spray	Hours	580	In range	± 80.00	Random Forest Regression	650	In range	550	In range	425	In range
10% Acetic acid submersion - 28 days	% wt	2.30	In range	± 0.40	Random Forest Regression	2.40	In range	2.10	In range	1.90	In range
Overall Matching		5/5				5/5		4/5		4/5	

Select Formulation(s)

Please Select ⌄

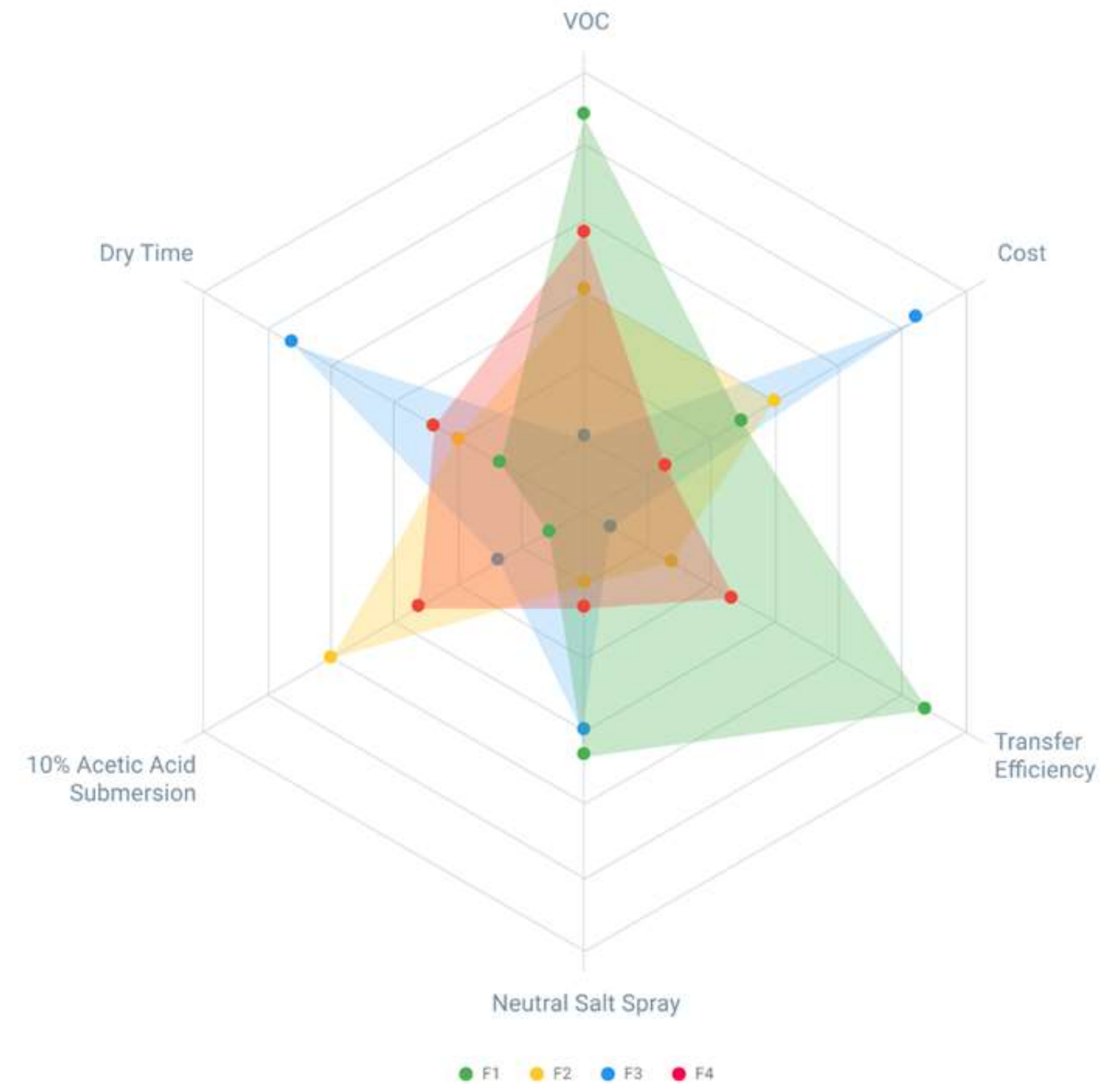# Detailed analysis and charting provides insight to inputs and outputs.

VOC / Neutral Salt Spray per Trial
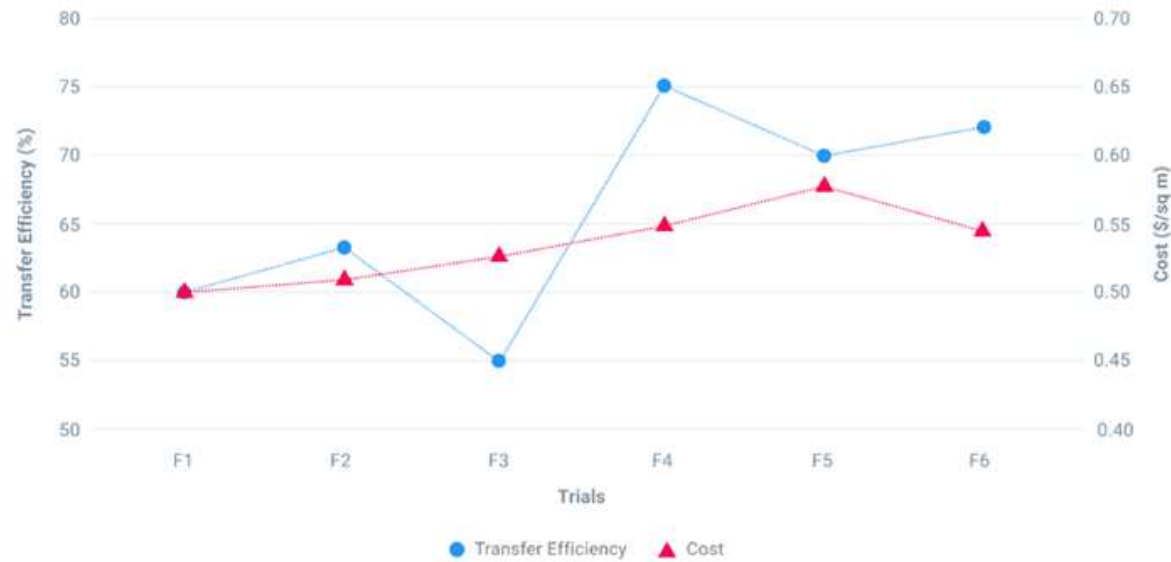
Property per Trial

Epoxide Resin Functionality / Neutral Salt Spray
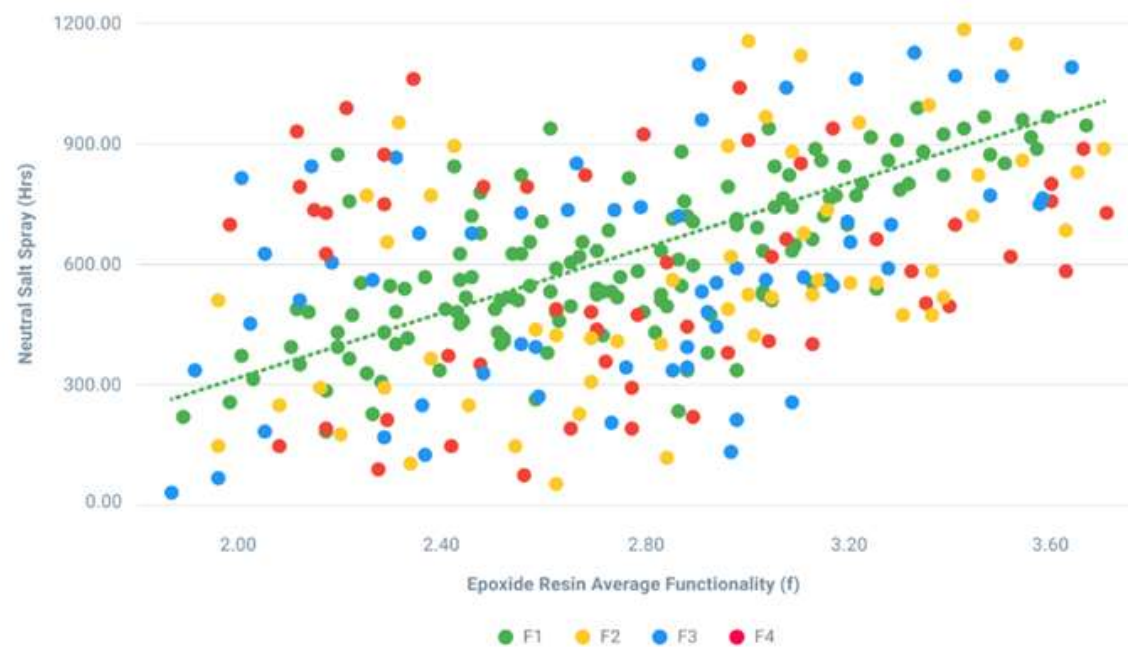
As well as detailed explanations of "why."

Neutral Salt Spray

Zinc Phosphate Neutral Salt Spray by +110 hours

EPON-1001-H-75 Neutral Salt Spray by +5 hours

DER 438 Neutral Salt Spray by +35 hours

- Relationships between
  - Materials
    (input parameters)
  - Impact on Performance
    (output parameters)

  can be visualized

- The magnitude of impact of each material is clear

Key Takeaways

- Every company will run AI

- Prioritize
  - Clean data capture
  - Data consolidation

- The right software can
  - Generate AI-ready data
  - Feed AI models at scale
  - Together, they will enable your AI efforts to scale across your organization

- Act with urgency as **<u>all</u>** AI learnings are valuable

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