

## **Executive Summary**



### **Current Al Adoption**

76% actively use AI in at least one discovery function. Top areas: Target ID/Validation (72%), Virtual Screening (68%), Preclinical/Tox modeling (61%), Lead Optimization (54%), Experimental Design (38%).



### **Realized & Projected Impact**

Current: 10–22% faster early discovery. By 2030: 30–50% shorter discovery/preclinical timelines; up to 45% cost savings in hit identification.



#### **Maturity Levels**

22% PoC only, 40% early implementation, 26% scaling across workflows, 6% fully integrated. Only ~1 in 3 organizations are scaling beyond pilots.



#### **Key Barriers to Scaling**

Data fragmentation (4.6/5), regulatory uncertainty (4.2/5), talent gaps (4.1/5), workflow integration (3.8/5), trust in Al design (3.5/5).



#### **Investment Priorities**

Shifting toward AI-ready data platforms, generative AI for chemistry/biology, ML-based decision support, partnerships with AI-native discovery companies, and workforce upskilling.

# **Current Al Adoption Across Discovery**

AI USE CASE	% OF ORGANIZATIONS
Target Identification & Validation	<b>72</b> %
Hit Discovery / Virtual Screening	68%
Early Preclinical Modeling & Toxicity Prediction	61%
Lead Optimization (e.g., generative ML models)	54%
Experimental Design & Automation	38%

## **Measured and Expected Impact**

### **Timeline Reduction Potential**





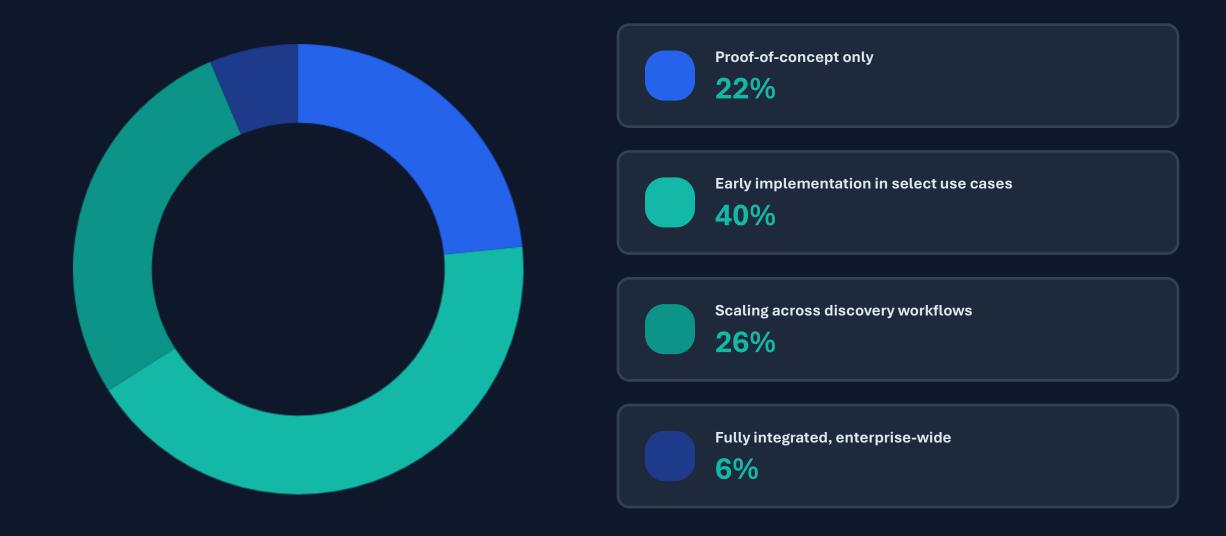
### **Cost Reduction Potential by Stage**

Hit Identification	
Current:	15–25%
<b>V</b>	
Ву 2030:	35–45%

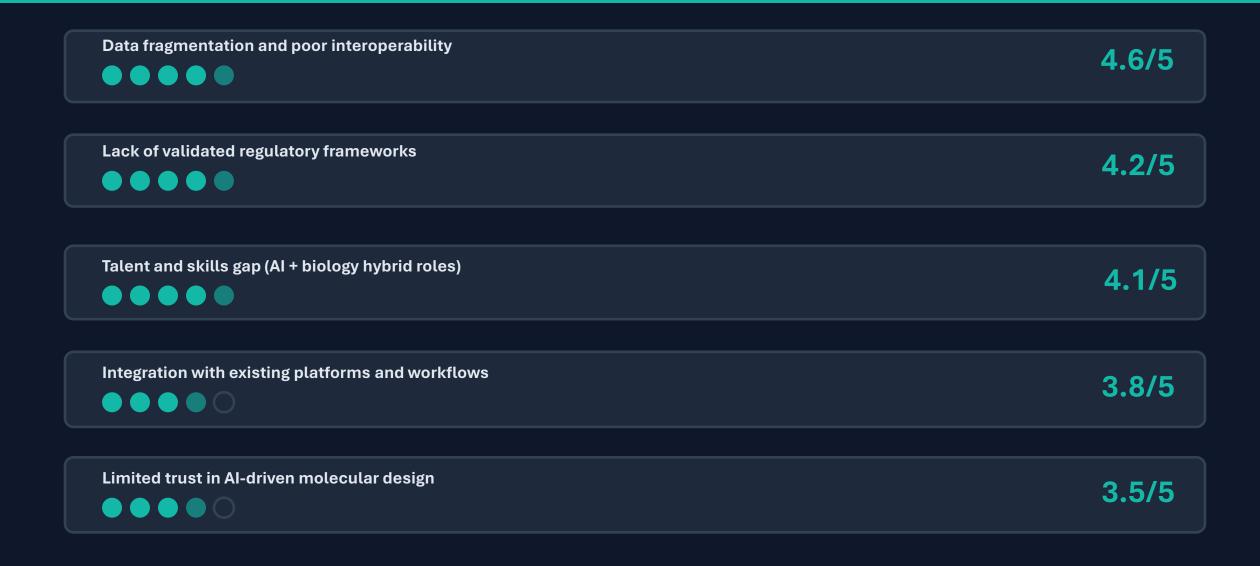
Lead Optimization	
Current:	10–20%
<b>V</b>	
Ву 2030:	25–40%

Toxicology & Preclinical Experiments		
Current:	5–15%	
<b>V</b>		
Ву 2030:	20–35%	

## **Maturity of Al Adoption**



## Key Barriers to Scaling AI in Drug Discovery



# Investment and Capability Focus

	Currently Investing	Planned in Next 24 Months
AI-Ready Unified Data Platforms	58%	76%
Generative AI for Chemistry/Biology	46%	71%
Automated / ML-Based Decision Support	34%	62%
Partnerships with Al-native discovery companies	<b>52</b> %	69%
Workforce Upskilling (Data + Bio R&D roles)	29%	57%

# **Future Outlook by 2030**

	Faster identification of novel targets	84%
	Higher probability of clinical success	72%
	Algorithm-driven molecular design replacing traditional screening	69%
	Significant reduction in lab-intensive experiments	61%
<b>✓</b>	Personalized/precision drug design	58%

## Quantitative Outlook at a Glance



**Active Al Adoption** 

68%

Organizations actively applying AI in chemical/biological design workflows

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Timeline Reduction by 2030

30-50%

Expected reduction in discovery timelines across the industry



**Hit Identification Savings** 

**Up to 45%** 

Cost savings projected in hit identification by 2030



**Lead Optimization Savings** 

25-40%

Cost reduction expected in lead optimization workflows



Al impact is strongest in early discovery and preclinical modeling, with higher probability of success entering clinical phases

## Final Insight

### Al is shifting from experimental to essential in pharma and biotech R&D



Scalable, Interoperable Data
Infrastructure



Regulatory Alignment and Validated Frameworks



Hybrid Talent: AI × Biology × Translational Science

### **Call to Action**

Invest now to operationalize AI across discovery and preclinical workflows. Organizations that build these capabilities today will define the next generation of drug discovery competitiveness.

