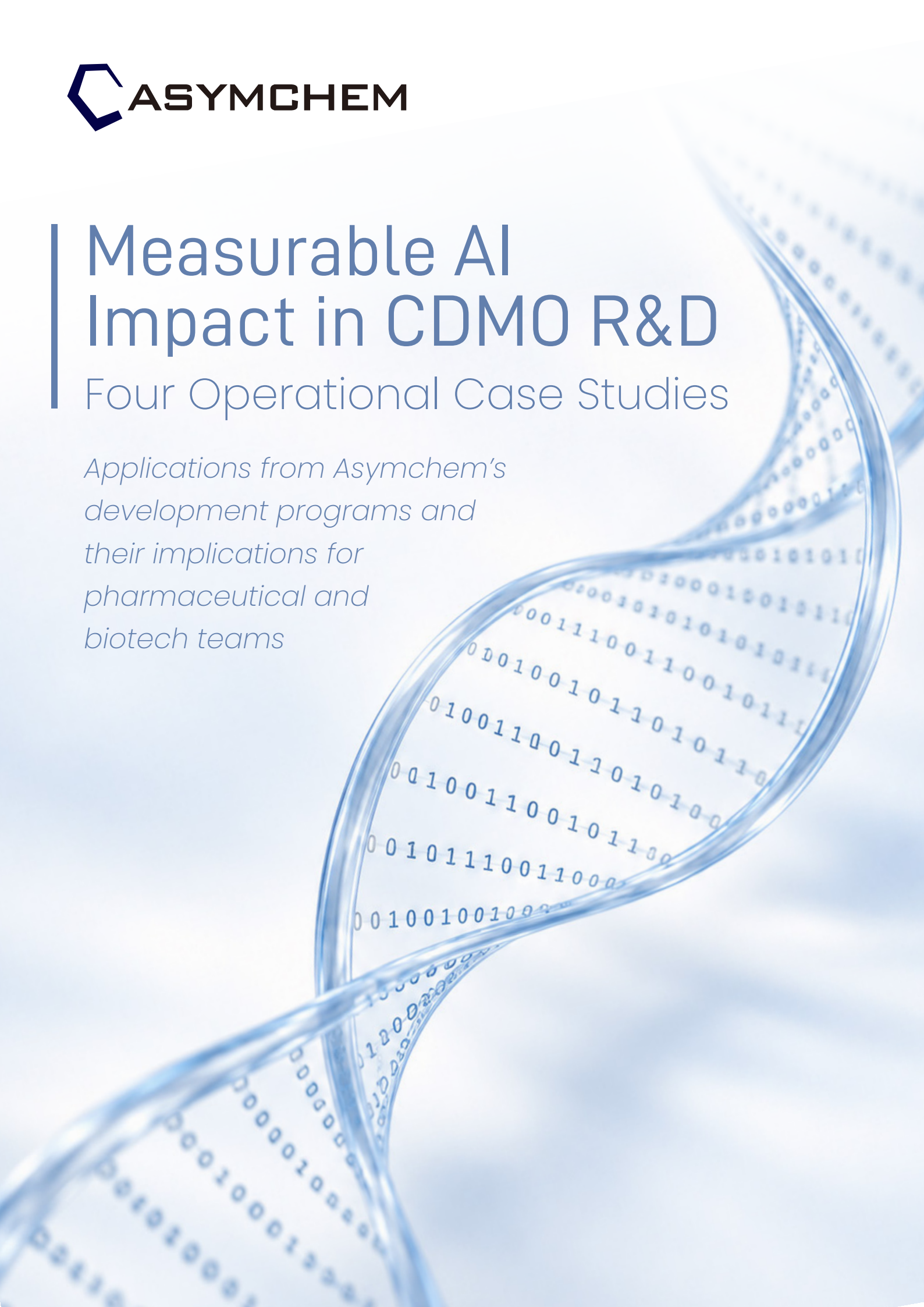
ASYMCHEM

Measurable AI Impact in CDMO R&D

Four Operational Case Studies

Applications from Asymchem's development programs and their implications for pharmaceutical and biotech teams



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Executive Summary

Artificial intelligence in the pharmaceutical industry has focused largely on drug discovery. Yet the most measurable returns today are emerging downstream in process development, analytical science, and manufacturing, where its impact can be evaluated using measurable operational outcomes.

This paper examines four operational AI deployments at **Asymchem**, a global CDMO, each selected based on the availability of quantifiable outcomes relative to a pre-AI baseline.

- **Enzyme engineering:** *Zymora*™, Asymchem's AI-assisted enzyme evolution platform, raised conversion from below 10% to over 80%, generating functional peptide ligases with less than 30% sequence identity to any natural enzyme.

- **Reaction development**: Machine learning models predicted amino acid racemization during peptide coupling with 86–90% accuracy and identified three dominant contributing factors. ML-assisted optimization was associated with yields above 90% across multiple projects.

- **Computational screening**: Virtual screening was used to eliminate poorly performing solvent and tag candidates computationally and to identify more sustainable solvents and reagents without additional experimental burden.

- **Impurity analysis**: Automated LC-MS annotation reduced impurity identification time from hours to minutes, corresponding to a fivefold efficiency gain; in one application, the insights supported a purity upgrade from 60% to 98%.

The common thread across these cases is not algorithmic sophistication alone, but the integration of AI with proprietary experimental data, mechanistic understanding, and institutional knowledge, a combination Asymchem refers to as *Asymchem Intelligence*. For pharmaceutical and biotechnology teams, these case studies illustrate how a development and manufacturing partner's AI capabilities can be evaluated quantitatively, using measurable outcomes such as development time, yield, and quality.



Industry Context: Rising AI Investment and the Evidence Gap

Few technologies have entered the pharmaceutical industry with expectations as high as those surrounding AI. The McKinsey Global Institute estimates that generative AI alone could unlock **$60–110 billion** in annual economic value for pharma and medical products.[1] Investment has risen accordingly: projected AI spending in life sciences nearly doubled in a single year, while adoption of agentic AI increased from 11% to 54%.[2]

Measured returns, however, have not kept pace. In November 2025, McKinsey reported that, despite the surge in investment, the industry has not seen substantially shorter development timelines or improved preclinical and clinical success rates.[3] Bain & Company quantified the gap: **only 20% of life sciences organizations are scaling AI with measurable value**, and the top-ranked barrier is human adoption, not technology.[4] For R&D and CMC leaders, the relevant question is therefore shifting from whether AI can provide value to where measurable value is being demonstrated, and under what conditions the results can be independently assessed.

Where value does appear, it tends to cluster in similar settings: large organizations with deep data infrastructure, knowledge-intensive tasks such as literature extraction and property prediction[5], and organizations with strong data foundations[6] — while regulators have begun formalizing what credible AI means.[7] The pattern is consistent: **AI delivers measurable results where three conditions coincide** — models tuned to specific industrial problems; proprietary experimental data accumulated over years; and workflows redesigned around AI.[3,5,6]

Implementing these conditions, and documenting the outcomes against defined baselines, remains the less common step. This paper examines what such implementation looks like in practice, through **four case studies from Asymchem**, whose operational AI deployments span enzyme engineering, reaction optimization, computational screening, and analytical science — downstream, regulated domains where published evidence remains limited. Each case is held to the same standard: an operational outcome, a stated baseline, and a lesson transferable to the wider industry.

About This Research

This paper draws on AI deployments in active development and manufacturing programs at Asymchem. Asymchem is examined as a case study, with cases selected according to three criteria: (1) the AI system is in operational use, not pilot stage; (2) outcomes are measurable against a pre-AI baseline; and (3) the underlying challenge is representative of problems common across the industry. Performance figures reflect Asymchem's internal project data; client-identifying information has been removed. Industry statistics are drawn from published third-party sources, cited throughout.

The paper is intended as an evidence-based perspective on industrial AI deployment, not a controlled comparative study.

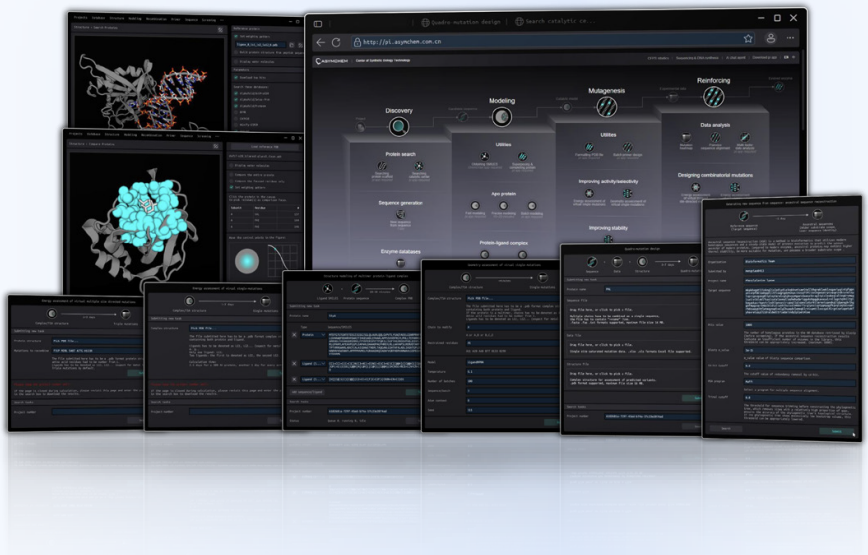
Case Study 1: Zymora™ & AI-Powered Enzyme Design

Technical challenge: Enzyme engineering can be a time-consuming stage of biocatalytic process development, and general purpose protein models, trained largely on public natural protein data, can face limitations when applied to the non-natural substrates and process conditions encountered in manufacturing. Peptide ligase development at Asymchem exemplified this challenge: more than 100 natural enzyme candidates were evaluated, and none achieved conversion above 10%.

Asymchem's approach: Asymchem redesigned the workflow around *Zymora*™, its AI-assisted enzyme evolution platform. *Zymora*™ fine-tunes foundation models on proprietary experimental data, mechanistic understanding, and accumulated project experience, identifying the most promising candidates computationally; laboratory effort concentrates on validating a short list. The platform has since been applied across enzyme classes — ketoreductases, hydrazone reductases, and oxidative cleavage enzymes — shortening timelines from concept development to ton-scale production.

Measured results: Conversion rate increased from less than 10% to greater than 80%. AI-guided design generated artificial peptide ligases with less than 30% sequence identity to any natural enzyme — sequences unlikely to have been identified through conventional natural-library screening.

Key takeaway: The principal outcome of this approach is a reduction in the number of experimental cycles required during early development, when the cost of each cycle is highest. For organizations evaluating a partner's enzyme engineering capability, a useful metric is the proportion of the candidate search that can be completed computationally before experimental work begins, rather than screening capacity alone.



Zymora

Asymchem's Next-generation AI-assisted Enzyme Evolution Platform

Case Study 2: Machine Learning for Reaction Development

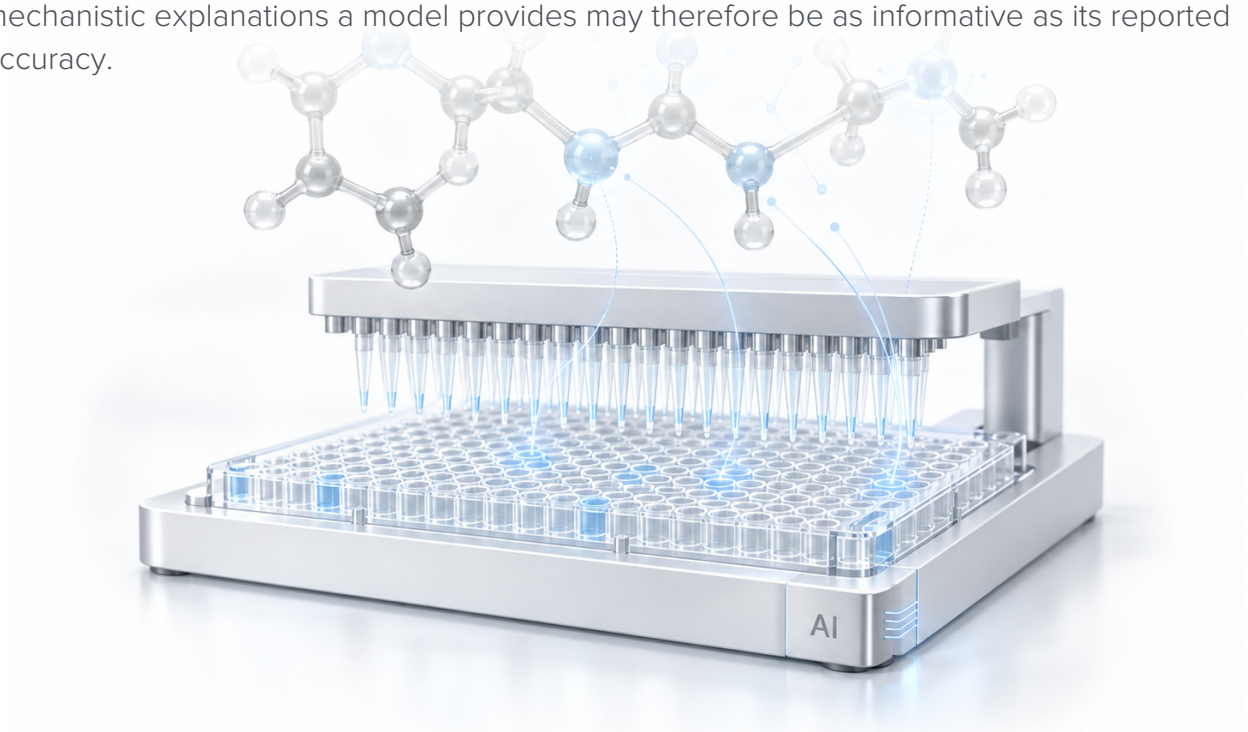
Technical challenge: Chemical process development is a combinatorial problem: choices of temperature, pressure, solvent, catalyst, and reagent multiply into thousands of possible conditions, rendering exhaustive experimental testing impractical.

In peptide synthesis, where coupling reactions alone yield tens of thousands of potential permutations, Asymchem targeted one of the most persistent quality risks: amino acid racemization during coupling.

Asymchem's approach: Asymchem applied its machine learning-assisted high-throughput reaction design platform to predict racemization outcomes before running experiments. The platform combines proprietary reaction datasets with quantum-chemistry-derived molecular descriptors, and the models — Gradient Boosting, Random Forests, and Bayesian Neural Networks — were selected for interpretability as well as accuracy, so that each prediction is accompanied by a mechanistic explanation.

Measured results: Prediction accuracy ranged from 86 to 90%. Model interpretation identified three dominant contributors: the properties of the activated ester, base strength, and solvent polarity. Across multiple projects, AI guided optimization identified reaction conditions that achieved yields above 90%, with reduced impurity formation and product racemization, as well as lower process costs.

Key takeaway: A distinguishing feature of this deployment is interpretability: a model that identifies why a condition fails generates transferable mechanistic insight rather than predictions alone. In evaluating machine learning approaches in process development, the mechanistic explanations a model provides may therefore be as informative as its reported accuracy.



Case Study 3: Computational Modeling and Green Chemistry

Technical challenge: Solvent and reagent selections have significant impacts on yield, purity, cost, and environmental footprint, yet it remains an experimentally intensive stage of process development.

In peptide manufacturing, solvent choice must simultaneously satisfy aggregation, solubility, stability, and purification requirements — a multi-objective problem where laboratory screening scales poorly. The same challenge appears in designing tag molecules for Asymchem's Tag-assisted Peptide Synthesis (TAPS) platform, where the search space spans large molecular libraries.

Asymchem's approach: Asymchem integrated molecular dynamics, molecular mechanics, quantum mechanics, and machine learning into a virtual screening workflow that evaluates molecular behavior before laboratory work begins. Machine learning performs the rapid first pass across large candidate libraries; quantum mechanical calculations then validate the shortlist. Poor candidates are eliminated computationally, and experimental effort is reserved for confirmation rather than exploration.

Observed impact: Poorly performing solvent and tag candidates are now eliminated in silico before laboratory work begins, and greener solvent and reagent choices are identified without additional experimental burden.

Key takeaway: As green chemistry becomes a criterion in outsourcing decisions, computational screening allows more sustainable solvents and reagents to be identified without additional experimental burden. A relevant consideration when assessing a partner is the proportion of solvent and reagent screening that is completed computationally before experimental work begins.



FASTER DISCOVERY
Shorten development timelines

HIGHER EFFICIENCY
Reduce experimental cycles

LOWER RISK
Improve success probability

GREATER IMPACT
Deliver more value to customers

Case Study 4: AI-Driven Impurity Annotation

Technical challenge: Modern analytical platforms generate LC-MS data faster than experts can interpret it. Manual impurity annotation can require hours of scientist time per analysis, creating a potential bottleneck in development programs and variability when interpretation differs among analysts.

In peptide development, impurity profiles are complex and the cost of misidentification is high: an unresolved impurity can stall process optimization or delay a batch decision. Asymchem needed impurity identification that was faster and less dependent on individual expert availability.

Asymchem's approach: Asymchem developed an automated LC-MS impurity annotation platform integrating sequence prediction, rule-based candidate generation, de novo sequencing, MS/MS spectrum prediction, retention time prediction, and automated scoring. Uploaded data is standardized, candidate impurities are generated and ranked against experimental spectra, and the scientist's role shifts from evaluating every possibility to reviewing a prioritized recommendation. Every completed annotation feeds back into a growing knowledge base.

Measured results: Annotation time was reduced from hours to minutes — an approximately fivefold efficiency gain. In one application, the resulting analytical and process insights supported a purity upgrade from 60% to 98%.

Key takeaway: Since impurity identification can be on the critical path of process changes and batch decisions, reducing analysis time from hours to minutes can shorten analytical turnaround time and support faster development decisions. The self-improving knowledge base also mitigates a widely recognized operational risk: the loss of expertise through staff turnover. A relevant consideration in evaluating an analytical platform is therefore whether its accumulated knowledge is retained and grows across projects.

The Prerequisite: Data Governance and Institutional Knowledge

The four cases share a common foundation that has less to do with algorithms than with infrastructure: data integrity, systematic knowledge capture, scientific governance, and organizational integration — assets that typically require sustained investment over many years.

The cases also illustrate a distinction worth naming — the one Asymchem draws between artificial intelligence and what it calls *Asymchem Intelligence*. Artificial intelligence provides the computational engine: the ability to learn, predict, classify, and optimize. *Asymchem Intelligence* refers to the integration of artificial intelligence with accumulated scientific knowledge, process understanding, proprietary data, and institutional experience. This integration enables general purpose algorithms to be applied within the context of chemical principles, process constraints, and regulatory requirements.

This foundation is maintained as a fully internal, closed-loop framework for core AI and R&D activities, with secure data governance and confidentiality standards designed around the trust pharma and biotech teams place in a CDMO partner. It also compounds over time: every case in this paper, from enzyme models trained on proprietary project data to an impurity platform that grows more capable with each annotation, returns new knowledge to the organization. General-purpose algorithms are becoming increasingly accessible; the proprietary data and institutional knowledge that make them effective are not.

Conclusion

This paper opened with a gap: an industry that has nearly doubled its AI budget in a single year, yet has limited evidence of shorter development timelines or improved success rates. The four deployments examined here do not close that gap for the industry, but they illustrate how it can be addressed at the level where results are generated — one program at a time, with outcomes quantified against a pre-AI baseline. None of these outcomes required a novel algorithm. Each depended on the same three conditions: a domain-specific model, proprietary data, and a workflow redesigned around prediction.

The implication for the industry is straightforward. The next phase of AI adoption is likely to be measured not in pilots launched or budgets approved, but in project-level results reported against stated baselines — evidence specific enough to be independently assessed. Organizations that report such evidence will help define what credible AI in drug development and manufacturing means, and teams that request it will be better positioned to capture its value.

About Asymchem

Asymchem (Stock Code: 002821.SZ/6821.HK) is a CDMO with more than 25 years of experience providing R&D and integrated production solutions across the pharmaceutical value chain.

Building on a foundation in small molecule CDMO services, the company has expanded its capabilities to encompass peptides, oligonucleotides, biologics, drug product, and clinical research services. Asymchem's capabilities continue to expand through technology development and transfer with a focus on continuous flow manufacturing and synthetic biology.

Asymchem operates R&D and manufacturing facilities in China, the United States, and the United Kingdom, and employs more than 9,000 professionals, approximately 45% of whom are dedicated to R&D. Asymchem partners with pharmaceutical and biotechnology companies worldwide and operate in accordance with applicable cGMP and EHS requirements across its development and manufacturing activities.

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