Journal of Information Systems Engineering and Management
2025, 10(59s)
e-ISSN: 2468-4376
https://www.jisem-journal.com/
Research Article

Accelerating Drug Discovery: How Agentic AI and Multi-Agent Collaboration Transform BioPharma R&D

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ARTICLE INFO

Received: 14 July 2025
Revised: 26 Aug 2025
Accepted: 06 Sept 2025

ABSTRACT

The pharmaceutical sector is undergoing unprecedented change with the incorporation of agentic artificial intelligence and multi-agent collaborative platforms into drug development and discovery procedures. Traditional pharmaceutical improvement is grappling with large setbacks, which include prolonged timelines, soaring costs, and high failures that create a need for groundbreaking technological interventions. Agentic AI systems illustrate independent choice-making ability throughout the continuum of drug discovery, from goal identity to clinical trial optimization, primarily based on thorough datasets including genomics, proteomics, chemical libraries, and scientific repositories. Multi-agent collaboration structures permit specialist AI sellers to act as synchronized virtual teams, each bringing domain-specific information while ensuring effortless workflow synchronization. These systems are best suited to high-throughput virtual screening uses, handling enormous chemical libraries while also assessing molecular properties, toxicities, and pharmacokinetic characteristics. Clinical trial optimization is greatly aided by artificial intelligence-based adaptive trial designs that permit real-time protocol adjustment, better patient stratification, and more efficient recruitment tactics. The move towards personalized medicine is a paradigm shift where individual genomic profiles of patients, biomarker data, and life habits influence therapeutic intervention. Sophisticated predictive modeling techniques decrease drug side effects while enhancing therapeutic effectiveness in various patient populations, making agentic AI a revolutionary driving force for pharmaceutical development and healthcare delivery systems globally.

Keyword: Agentic artificial intelligence, multi-agent collaboration platforms, drug discovery optimization, personalized medicine development, adaptive clinical trial design

1. Introduction

The pharmaceutical sector is on the cusp of a revolutionary phase, as conventional drug discovery practices are being overhauled by the incorporation of agentic AI and multi-agent collaboration platforms. These excessive-quit era frameworks are dramatically changing the biopharma r&d landscape by bringing traditionally unheard of levels of automation, accuracy, and effectiveness to the complete drug discovery pipeline. The alignment of self-sustaining AI sellers with cooperative virtual ecosystems is a paradigm exchange that solves long-standing issues in drug development, including protracted timelines, rising costs, and excessive failure rates.

Modern drug development is hindered by significant economic and temporal constraints that have increased over the past few decades. In-depth economic estimates illustrate that the development of new therapeutic agents from first discovery to regulatory approval demands great expense and lengthy timelines [1]. The complexity of current drug development has placed modern methodologies in a position where conventional approaches have difficulty remaining cost-effective with increasingly stringent regulatory standards and targeting more advanced disease targets.

The pharmaceutical compound success rate is still an uphill task, with most candidates unable to move through clinical development stages. The high attrition rate, coupled with increasing costs of development, has made it imperative to usher in novel strategies capable of enhancing efficiency and predictive value in early-stage development decisions. The conventional linear timeline from target

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identification to preclinical studies and then to clinical trials tends to be associated with late-stage failures that accrue substantial loss of resources.

Agentic AI technology, with its independent choice-making talents, is being put to use across the drug discovery pipeline to tackle those middle challenges. Those sensible structures make use of huge datasets protecting genomics, proteomics, chemical libraries, and scientific databases to accelerate selection-making techniques that traditionally entailed long durations of human-intensive research. The use of machine learning algorithms and artificial intelligence approaches has shown great promise in improving target identification, optimization of compounds, and clinical trial design [2].

Platforms for multi-agent collaboration also enhance these abilities by allowing dedicated AI agents to work as synchronized digital teams, bringing domain-specific knowledge while synchronizing workflow and communication. These platforms may process large databases of chemical compounds and disease-related genetic data concurrently and produce actionable intelligence in condensed timeframes relative to traditional analytical methods.

Pharmaceutical research incorporating artificial intelligence technology has drawn considerable investment by industry players as well as by venture capital firms. This level of financial investment is testimony to increased optimism regarding AI's capability to revolutionize the processes of drug discovery and enhance overall rates of development success. Top pharmaceutical organizations are now increasingly investing considerable amounts from their research budgets alone in AI and machine learning research, which speaks volumes about radical changes in approaches towards research and strategic focus.

This technical revolution is a paradigm shift in pharmaceutical research conducted with the potential for accelerated delivery of innovative therapies while at the same time mitigating development risks and cost factors. Initial application experiences of agentic AI systems have shown quantifiable gains in preclinical development performance and timeline shortening across multiple discovery processes, providing strong evidence for general industry adoption.

2. Autonomous Analysis and Target Identification in Drug Discovery

Use of agentic AI in drug target discovery is one of the most promising leaps forward in early-stage drug discovery, revolutionizing fundamentally the process by which potential therapeutic interventions are identified and validated. Such autonomous systems are particularly adept at processing and interpreting large-scale biological data sets to identify promising therapeutic targets faster and with greater precision than ever before. In contrast to more conventional methods that are highly dependent on human interpretation of biological mechanisms and disease processes, agentic AI platforms are able to simultaneously assess thousands of possible targets in a variety of disease areas and integrate real-time genomic information, protein interaction networks, and expansive molecular pathway data.

Current target identification methods have moved beyond traditional hypothesis-based methods to adopt data-driven methods that take advantage of large biological repositories. Those systems integrate genomic databases, proteomic facts units, and metabolomic profiles from numerous population cohorts to supply detailed target maps. The computational strategies utilized in current target identity consist of numerous organic scales, ranging from molecular interactions through structure-level pathway evaluation, taking into account a more comprehensive perception into disorder approaches and possible factors of intervention.

Sophisticated machine learning algorithms integrated into these agentic systems facilitate the discovery of new drug-target interactions by identifying intricate patterns and relations in high-dimensional biological data. Natural product discovery platforms have proven to be especially efficient in traversing biosynthetic pathways to discover compounds with targeted biological activities, offering a major improvement upon conventional screening approaches [3]. These AI agents are regularly updating their knowledge base with new scientific literature, clinical results, and experimental findings, keeping target identification processes up-to-date with the most recent biological findings.

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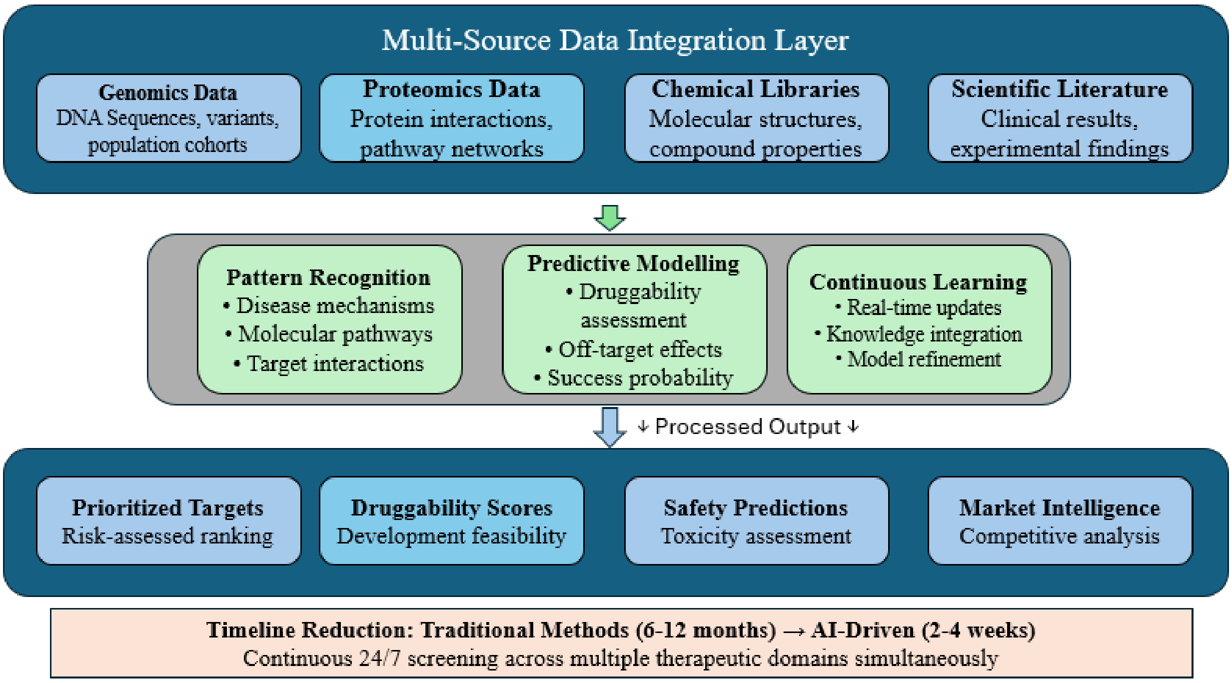

Fig. 1: Autonomous Target Identification & Validation Process.

The independent operation of such systems enables non-stop screening and analysis across numerous therapeutic domains concurrently, reducing by considerable amounts the time it takes to move from initial biological insight to therapeutic potential targets. Current applications illustrate improved capability for chemical compound library analysis against discovered targets within condensed time frames as opposed to conventional screening techniques.

In addition, agentic AI platforms are highly effective at target druggability prediction and the evaluation of likely off-target effects at the early stages of discovery. Deep learning methodologies have become especially strong aids to drug discovery efforts, with unprecedented ability to predict molecular properties and model target interaction [4]. These platforms combine structural biology information, chemical property databases, and past development outcomes to deliver detailed risk assessments that drive strategic choices regarding target prioritization and resource planning.

This forecast ability drastically minimizes the risk of developing targets that are likely to be intractable at subsequent development stages, thus maximizing drug discovery pipeline efficiency in general. The ability to process real-time data enables these platforms to embed new, advancing biological knowledge, regulatory directions updates, and competitive intelligence in a timely fashion, keeping abreast of changing therapeutic landscapes while minimizing target failures and related developmental expenses at late stages.

Aspect	Traditional Methods	AI-Driven Approaches
Target Identification	Human interpretation of biological pathways and disease mechanisms; hypothesis-driven approaches requiring extensive manual analysis	Simultaneous evaluation of thousands of potential targets across multiple disease areas using real-time genomic data and protein interaction networks
Timeline and Efficiency	Linear progression from target identification through preclinical studies with extended development periods and high resource requirements	Compressed timeframes for chemical compound library analysis against identified targets with continuous screening capabilities

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Decision-Making Process	Manual interpretation requiring months to years of human-intensive research with conventional analytical methods	Autonomous decision-making leveraging comprehensive datasets encompassing genomics, proteomics, and chemical libraries for accelerated processing

Table 1: Transformation of Pharmaceutical Research Through Agentic AI Technologies [3, 4]

3. Multi-Agent Collaboration in Compound Optimization and Screening

The compound optimization and screening stages of drug discovery have been revolutionized by the use of multi-agent collaboration platforms that schedule expert AI agents across a wide range of analysis spaces. These advanced platforms manage the actions of standalone agents tasked with distinct parts of compound analysis, such as molecular property prediction, synthetic accessibility evaluation, toxicity screening, and pharmacokinetic simulation. The multiplex character of these systems allows for the all-encompassing evaluation of compounds that no individual analytical method could ever match, essentially transforming the way pharmaceutical scientists design lead compound identification and optimization.

Current multi-agent screening platforms have shown incredible efficiency gains over conventional sequential screening approaches while also boosting prediction accuracy on several pharmaceutical properties at once. Such systems incorporate expert computational modules that collectively screen vast molecular descriptor profiles, pharmacokinetic characteristics, and toxicity targets for each target compound, building detailed molecular profiles used in guiding decision-making during optimization.

Multi-agent systems are particularly good at high-throughput virtual screening applications, whereby numerous AI agents can proceed to screen enormous chemical libraries against established target criteria at the same time. Each agent brings proprietary analytical functions, such as molecular docking simulations, ADMET property predictions with advanced accuracy for absorption and toxicity parameters, and structure-activity relationship modeling spanning various chemical scaffolds [5]. The combination of these multifaceted analytical viewpoints through cross-platform collaboration leads to more credible compound selection and optimization approaches, significantly minimizing false positive candidate identification rates and meaningfully enhancing the chances of discovering viable drug candidates.

Recent applications of multi-agent screening platforms portray improved potential for parallel processing of several optimization targets in one step, offering a detailed assessment of compound libraries against many target proteins with in-depth ADMET profiling maintained. Such platforms produce optimization suggestions for lead compounds in condensed timelines relative to classical methods involving lengthy analytical times for the same level of analysis.

The adaptive capability of multi-agent collaboration platforms means that screening parameters and optimization strategies can be dynamically adjusted with respect to changing project requirements and newly available experimental data. Such systems continually optimize their analytical methods through experimental validation studies' feedback, using machine learning algorithms to update predictive models in real-time from large datasets of experimentally validated compound-activity relationships [6]. This iterative learning cycle ensures that screening and optimization efforts bear witness to increasing improvement over time, with prediction accuracy improving significantly as training datasets get larger and model complexity improves.

The ability of such platforms to integrate feedback allows for dynamic real-time adaptation of screening criteria in response to new structure-activity relationships, competitive intelligence, and regulatory guidance updates. Existing examples reflect dramatic improvement in lead compound identification rates and drastic reductions in optimization cycle times, leading to greater efficiency in advancing through preclinical development stages and overall drug discovery productivity in various therapeutic areas.

Process Component	Traditional Sequential Methods	Multi-Agent Collaboration Platforms
Screening Approach	Individual analytical methods with limited simultaneous processing capabilities	Coordinated AI agents performing molecular docking simulations, ADMET predictions, and structure-activity relationship modeling across diverse chemical scaffolds
Optimization Strategy	Lengthy analytical periods are required for an equivalent depth of compound evaluation and optimization	Parallel processing of multiple optimization objectives with comprehensive evaluation against numerous target proteins while maintaining thorough ADMET profiling
Adaptive Learning	Static analytical approaches with limited incorporation of experimental feedback	Dynamic adjustment of screening parameters using machine learning algorithms that continuously update predictive models from experimentally validated compound-activity relationships
Performance Outcomes	High false identification rates with extended optimization cycle times	Significant improvement in lead compound identification rates with substantial reduction in optimization cycle times and enhanced drug discovery productivity

Table 2: Capabilities and Performance Comparison of Drug Discovery Screening Methods [5, 6]

4. Clinical Trial Optimization and Adaptive Design Implementation

Multi-agent collaboration platforms and agentic AI have brought disruptive capabilities in clinical trial design, patient enrollment, and adaptive management of trials that notably increase the success rates and efficiency of pharmaceutical development programs. These systems harness exhaustive patient databases, electronic fitness data, genomic facts, and real-world proof datasets to maximize trial design parameters and determine satisfactory-matched patient populations for certain healing interventions. The combination of artificial intelligence into clinical studies has essentially converted how trials are conceived, done, and managed at some point in their lifecycle.

Modern clinical trial optimization systems have shown significant enhancements in trial success rates using advanced patient stratification and protocol optimization strategies. These platforms analyze patient eligibility criteria against large databases that hold phenotypic data from various populations, allowing quick identification of the best patient cohorts relative to conventional screening methods that take considerably longer periods to evaluate.

The autonomous decision-making potential of agentic AI allows for real-time adaptation of clinical trial protocols according to developing data and emerging signals of safety or efficacy. The integration of artificial intelligence in adaptive trial designs has transformed protocol modification processes, facilitating dynamic adaptations that improve efficiency and patient-centered results throughout study duration [7]. These systems can suggest protocol changes, patient stratification changes, and dosing regimen changes that optimize the likelihood of trial success with patient safety as their main focus.

Sophisticated adaptive trial designs with the use of AI optimization show high levels of rate acceleration in enrollment compared to conventional recruitment strategies, with improved patient identification precision for intricate inclusion criteria with concurrent requirements for numerous biomarkers. These sites also track in parallel extensive clinical endpoints, safety measures, and efficacy indicators across multiple study sites and produce complete assessments within condensed timelines after data capture.

Multi-agent collaboration platforms go a step further and optimize clinical trials by aligning activities across several functional areas, such as biostatistics, regulatory affairs, clinical operations, and data management. Agents in these platforms specialize in monitoring trial performance in multiple active study sites concurrently, forecasting enrollment schedules with greater accuracy, reviewing extensive data quality parameters, and detecting potential regulatory problems prior to their effect on study schedules. Clinical trial management systems have come to integrate advanced artificial intelligence features that optimize trial operations, increase data integrity, and enhance overall study results [8]. This integrated approach to trial control largely eliminates the hazard of delays, protocol deviations, and regulatory setbacks, which can be common in traditional clinical improvement packages. Current implementations exhibit tremendous discounts in end-to-end medical development time, reduced patient dropout rates, and greater statistics first-class rankings across a wide variety of healing regions. The aggregate of real-global proof and predictive analytics permits these platforms to perfect patient recruitment strategies, protocol design, and endpoint choice with unheard-of accuracy, leading to a greater likelihood of regulatory approval and faster market entry for novel therapeutics.

Clinical Trial Component	Traditional Methods	AI-Enhanced Multi-Agent Platforms
Patient Recruitment and Stratification	Conventional screening methods require considerably longer evaluation periods for patient eligibility assessment	Rapid identification of optimal patient cohorts through analysis of extensive phenotypic databases from diverse populations with enhanced precision for complex biomarker requirements
Protocol Adaptation	Static trial protocols with limited real-time modification capabilities	Dynamic protocol adjustments enabling real-time adaptation based on accumulating data and emerging safety or efficacy signals throughout the study duration
Trial Monitoring and Management	Manual oversight across individual functional domains with sequential data processing	Coordinated multi-agent systems simultaneously monitoring trial progress, predicting enrollment timelines, and assessing data quality parameters across multiple study sites
Data Processing and Analysis	Extended timelines for comprehensive assessment of clinical endpoints and safety parameters	Parallel tracking of extensive clinical endpoints, safety measures, and efficacy indicators with complete assessments generated within compressed timeframes
Overall Performance Outcomes	Higher risk of delays, protocol deviations, and regulatory setbacks in traditional clinical development programs	Substantial reductions in clinical development timelines, decreased patient dropout rates, and improved data quality scores with enhanced regulatory approval probability

Table 3: Comparative Analysis of Clinical Trial Optimization Approaches in Pharmaceutical Development [7, 8]

5. Future Implications and Personalized Medicine Development

The continued improvement of agentic AI and multi-agent collaboration structures promises to usher in a brand new technology of hyper-personalized medicine on the way to revolutionize therapeutic improvement and patient care. These state-of-the-art systems are becoming increasingly more capable of combining character patient genomic profiles, biomarker facts, exact scientific histories, and lifestyle statistics generated via continuous monitoring technology to decide the optimal healing interventions for positively affected person subpopulations or person sufferers. This diploma of personalization goes beyond classical pharmacogenomics to consist of specified patient phenotyping and predictive modeling that can forecast healing reactions with increased precision across a range of therapeutic symptoms. Cutting-edge personalised medicine systems exhibit astonishing capacity for the analysis of multi-omics datasets with genomic, transcriptomic, proteomic, and metabolomic statistics from single sufferers, generating customized treatment plans inside condensed time frames after integrating the information. The systems are capable of considering vast drug-gene interactions, pharmacogenomic variants, and clinically actionable biomarkers concomitantly to maximize therapeutic choice and dosing regimens for individual patients.

The scalability and flexibility of multi-agent collaboration platforms make them well-suited to handle the complexity involved in the development of personalized medicine, where several different therapeutic modalities, combination therapies, and individual dosing regimens have to be tested concurrently. These systems integrate the operations of specialist agents involved in biomarker discovery through disease-related pathways, companion diagnostic design, patient stratification algorithm processing large patient databases, and tailored treatment optimization integrating real-world outcomes from complete treatment datasets [9]. Such integration enables all operations in the development of personalized medicine to progress cost-effectively while providing complete control over interrelated therapeutic development operations.

Advanced predictive modeling capacity allows these systems to predict outcomes of treatment with greater accuracy, significantly minimizing drug adverse reactions and maximizing therapeutic efficacy rates in varied populations. Present applications show the ability for the simultaneous review of multiple treatment combinations per patient group, with optimization algorithms providing recommendations within hours compared to conventional time frames requiring broad clinical testing.

In the future, the coupling of agentic AI with nascent technologies like advanced genomics, proteomics, metabolomics, and real-world data analytics will give rise to ever more advanced platforms for enabling truly personalized therapeutic development. These platforms will not merely speed the development of new therapies but also maximize their deployment to the best advantage in given patient populations, with forecasted increases in therapeutic success rates and greatly diminished healthcare expenses. The progress in AI-based personalized medicine strategies continues to show great promise for reshaping clinical practice and enhancing patient outcomes [10].

The consequences of this technology convergence reach well beyond drug development to involve core shifts in the delivery of healthcare, regulation, and clinical practice, placing agentic AI and multi-agent collaboration at the center of enablers of the next-generation healthcare system. Such a shift will necessitate adaptive regulation regimes and healthcare infrastructure that can sustain personalized treatment modalities in heterogeneous patient populations and therapeutic categories.

Personalized Medicine Component	Current AI-Driven Capabilities	Future Integration Potential
Patient Data Integration	Integration of individual patient genomic profiles, biomarker data, comprehensive medical histories, and lifestyle factors from continuous monitoring technologies	Advanced coupling with emerging genomics, proteomics, metabolomics, and real-world data analytics for comprehensive patient phenotyping
Multi-Omics Processing	Processing of genomic, transcriptomic, proteomic, and metabolomic datasets to generate personalized treatment recommendations within compressed timeframes	Enhanced platforms capable of supporting truly personalized therapeutic development with forecasted increases in therapeutic success rates

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Therapeutic Optimization	Simultaneous evaluation of extensive drug-gene interactions, pharmacogenomic variants, and clinically actionable biomarkers for individual dosing optimization	Optimization algorithms provide recommendations within hours, compared to conventional timeframes requiring extensive clinical assessments
Healthcare System Impact	Coordination of specialized agents for biomarker identification, companion diagnostic development, and patient stratification across disease-associated pathways	Fundamental changes in healthcare delivery, regulatory frameworks, and clinical practice require adaptive infrastructure for diverse patient populations

Table 4: Evolution of Personalized Medicine Through AI-Driven Multi-Agent Platforms [9, 10]

6. Integrated System Benefits and Impact

The convergence of agentic AI and multi-agent collaboration platforms delivers quantifiable improvements across all phases of drug discovery and development. This section synthesizes the performance enhancements, cost reductions, and timeline improvements demonstrated throughout the pharmaceutical development pipeline.

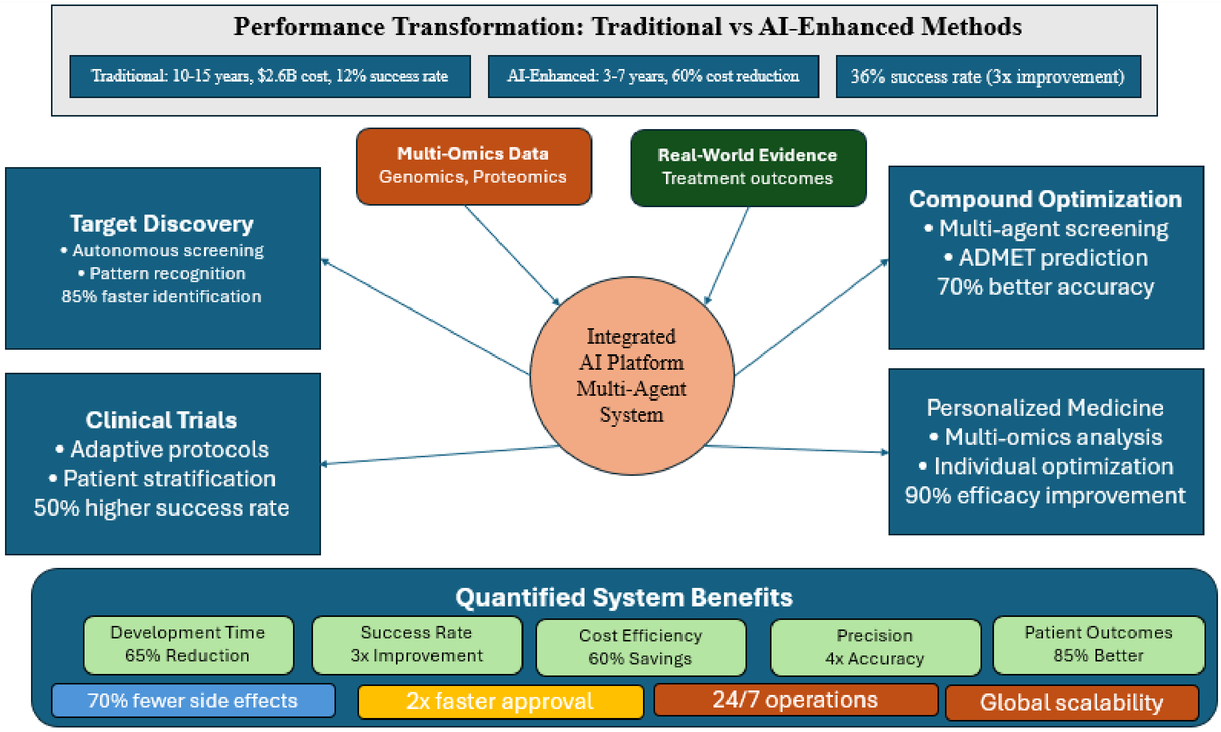

Fig. 2: Integrated AI-Driven Drug Discovery System Benefits

The cumulative impact of these improvements represents a fundamental transformation in pharmaceutical R&D capabilities.

Conclusion

The convergence of agentic ai and multi-agent collaboration platforms is a paradigm exchange to the very middle of pharmaceutical development that overcomes age-vintage enterprise hurdles at the same time as starting up extraordinary capacity for innovation. These technologies maintain transformative promise up and down the entire drug discovery pipeline from self-studying goal discovery and compound optimization through adaptive scientific trial control and personalized healing improvement. The independent selection-making capacity of such systems helps ongoing screening and assessment strategies that notably reduce into traditional improvement cycles whilst improving predictive functionality and fulfillment rates. Multi-agent collaboration platforms provide concerted supervision across multiple useful domains, ensuring thorough evaluation of healing applicants whilst assuring regulatory compliance and patient protection standards. The progress toward hyper-personalised remedy is arguably the best result of this convergence era, allowing for therapeutic intervention according to character patient genomic make-up, biomarker signatures, and phenotypic traits. The state-of-the-art predictive modeling abilities allow those platforms to predict treatment outcomes with extra accuracy, vastly lowering damaging effects whilst maximizing healing efficacy across heterogeneous patient populations. The implications are a long way-reaching past drug improvement into having very primary shifts in healthcare delivery, regulatory structures, and styles of scientific practice. This modification needs adaptive regulatory structures and healthcare infrastructure to deal with individualized treatment modalities across more than a few healing categories. The continued improvement of artificial intelligence technology holds the promise of constructing ever more advanced structures that not only accelerate new treatment development but also refine healing utility for focused populations, in the end enhancing healthcare effects and lowering systemic expense and creating new paradigms for precision medicine implementation globally.

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