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AI-Enabled Drug Candidates and the Evolving Role of CROs

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Abstract: The integration of artificial intelligence (AI) into early-stage pharmaceutical research is fundamentally reshaping the landscape of drug discovery. From generative chemistry and predictive modelling to phenotypic screening and target identification, AI is accelerating timelines, reducing attrition, and enabling a new class of clinical candidates. This paradigm shift has significant implications for contract research organizations (CROs), which are evolving from traditional service providers into strategic partners in data-driven discovery. In this paper, we examine the rise of AI-native drug candidates, analyse their journey from code to clinic, and explore how contract research organizations (CROs) are adapting their infrastructure, capabilities, and business models to remain competitive. Through case studies of companies, the transformative potential of CRO–AI biotech collaborations is illustrated. Also addressed were the regulatory, ethical, and operational challenges facing CROs, and a forward-looking perspective was provided on how they can capture value in an AI-enabled future.

Keywords: artificial intelligence, drug discovery, contract research organizations, AI-designed drug candidates, generative models, CRO–Biotech collaboration, machine learning, pharmaceutical innovation.

INTRODUCTION

ARTIFICIAL intelligence (AI) has emerged as one of the most transformative forces in the pharmaceutical industry, revolutionizing the way new drugs are discovered, optimized, and advanced into clinical testing.[1] Over the past decade, AI has shifted from a theoretical frontier to a practical and increasingly indispensable element of early-stage research. By enabling the design of novel chemical matter, predicting biological activity, simulating pharmacokinetic profiles, and streamlining compound selection, AI is accelerating discovery timelines and reducing attrition in ways that were previously unthinkable.[2] Artificial intelligence is now seen as a general-purpose technology with far-reaching implications across biomedical research, similar to the transformative roles of electricity and the internet in earlier eras. However, AI models are only as good as the data on which they are trained; biases in datasets, particularly those underrepresenting diverse populations, can propagate inequities and hinder true translational progress. As a result of these changes, the traditional research and development (R&D) ecosystem is undergoing a profound realignment. Contract Research Organizations (CROs), which have historically operated as external laboratories and service providers, are now being drawn into the core of discovery innovation. The rise of AI has not only shifted the nature of work performed but has also created new expectations around data quality, speed, and strategic collaboration. AI-enabled biotech companies require CROs to do more than execute protocols, they need them to become data partners, validation engines, and innovation enablers.[3,4]

This paper examines the current and future roles of CROs in the era of AI-enabled drug discovery. It examines how the integration of machine learning models into the design–make–test–analyse (DMTA) cycle is reshaping scientific workflows and identifies the technological, operational, and cultural shifts CROs must undergo to remain competitive. Case studies from industry leaders are used to illustrate both the promise and the complexity of this new paradigm.

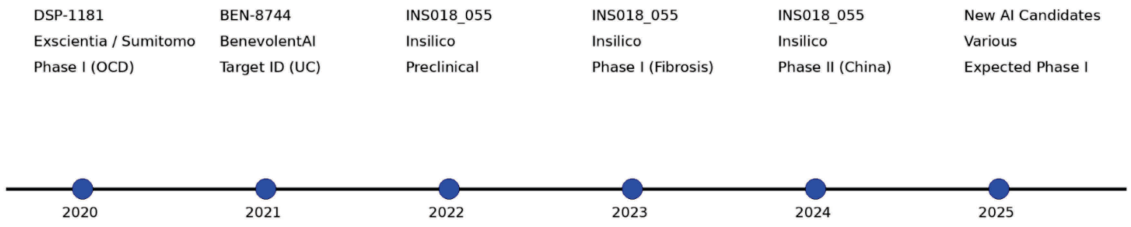

Figure 1. Timeline of AI-Designed Drug Candidates Advancing into Clinical Trials (2020–2025).

AI-Driven Transformation of Drug Discovery and the Role of CROs

AI has steadily moved from the periphery to the centre of drug discovery, catalysed by the convergence of computational power, algorithmic advances, and the availability of large-scale biological and chemical datasets. Traditional discovery methods, which rely on high-throughput screening and iterative medicinal chemistry, are increasingly being complemented, and in some cases, replaced by deep learning models that predict target binding, optimize molecular properties, and simulate biological outcomes.[4]

The first tangible milestones of this transition appeared in 2020, when Exscientia's AI-designed molecule DSP-1181, developed in partnership with Sumitomo Dainippon Pharma, became the first AI-generated drug to enter Phase I clinical trials.[5,6] This was followed by Insilico Medicine's fibrosis-targeting INS018_055, which completed Phase I trials in China in 2023 and moved into Phase II.[7,8] BenevolentAI also advanced a candidate for ulcerative colitis (BEN-8744) to clinical trials, using AI to identify a novel target and optimize the compound series.[9,10] A timeline of key AI-designed candidates entering the clinic is provided in Figure 1. This timeline highlights key milestones for the first generation of AI-discovered or AI-designed drug candidates. Several new AI-native candidates are expected to reach Phase I globally by the end of 2025.

A comparative overview of selected AI-designed clinical candidates is provided in Table 1. This table presents a selection of prominent drug candidates generated or optimized using artificial intelligence methodologies. The list includes compounds at various clinical stages, discovered by AI-first or AI-integrated biotech companies such as Exscientia, BenevolentAI, and Insilico Medicine. Insilico integrated platform spans generative chemistry, target discovery, and even virtual clinical trial simulations, compressing timelines and iteratively refining candidate profiles. Highlighted is the increasing role of AI in progressing molecules from virtual design to human trials, as well as the involvement of CROs in executing preclinical and early clinical activities.[1,11]

Table 1. Representative AI-Designed Drug Candidates in the Clinic.

MOLECULE	COMPANY	TARGET INDICATION	CLINICAL PHASE	CRO PARTNER(S)
DSP-1181	Exscientia / Sumitomo	Obsessive-Compulsive Disorder	Phase I	Evotec
BEN-8744	BenevolentAI	Ulcerative Colitis	Phase I	Not disclosed
INS018_055	Insilico Medicine	Fibrosis	Phase II	Local (China/NZ)
New AI Candidates	Various	Various (TBD)	Expected Phase I	To be announced

Generative chemistry models, such as variational autoencoders (VAEs), generative adversarial networks (GANs), and transformer-based architectures, now enable the de novo design of drug-like molecules optimized for multiple objectives. [12,13,14,15] Predictive models, based on graph neural networks, ensemble learning, and support vector machines, help triage virtual libraries, predict bioactivity, and flag various Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) liabilities. These models are embedded in iterative feedback loops that connect in silico hypotheses with in vitro and in vivo results.[16,17]

AI also plays a critical role in target identification. Natural language processing (NLP) tools, such as BioBERT, and proprietary algorithms used by companies like BenevolentAI, mine biomedical literature, electronic health records, and clinical trial databases to discover new disease–target associations.[9–11] Structure-based design has been revolutionized by AlphaFold and its successors, enabling modelling of previously "undruggable" proteins. AlphaFold has transformed structural biology by predicting protein structures with near-experimental accuracy, dramatically accelerating the pace of target validation and structure-based drug design.[18,19] In parallel, integrative tools such as Scanorama enable the merging of heterogeneous datasets, such as single-cell transcriptomes, thereby enhancing the granularity and effectiveness of target discovery.[40] Crucially, these tools are no longer the exclusive domain of large pharma companies. A growing class of AI-native biotech like Atomwise, Valence, and

Genesis Therapeutics now designs candidates almost entirely in silico and relies on CROs for rapid, high-quality experimental testing.[20–22] This evolving division of labour is reshaping the landscape of drug discovery, expanding both the methods employed and the range of contributors involved. By transcending traditional mechanistic reasoning, AI enables hypothesis-free discovery through the detection of hidden patterns within complex, high-dimensional, and multimodal datasets.

AI-enabled discovery is shifting drug R&D from a linear, siloed process to an adaptive, iterative paradigm. Traditionally, discovery progressed in discrete phases: target identification, hit generation, hit-to-lead optimization, and preclinical validation. Each phase was executed independently, often by different teams or vendors, with long delays between steps. [1,2,20,23] By contrast, AI facilitates continuous and rapid iteration. The DMTA cycle is now driven by real-time model updates based on feedback from experiments. Machine learning algorithms suggest compound modifications, CROs synthesize and test the compounds, and new data are fed back into the model within days or even hours.[24,25] This accelerates learning, narrows chemical space efficiently, and reduces the risk of late-stage failure.

The transformation of the DMTA cycle into a closed-loop AI-enabled process is illustrated in Figure 2. This schematic illustrates how artificial intelligence integrates into the iterative Design–Make–Test–Analyse (DMTA) cycle. AI-based generative models propose new molecular structures (Design), which are synthesized by CROs or automated platforms (Make), followed by experimental evaluation through biochemical, phenotypic, or ADMET assays (Test). The resulting data feeds back into predictive and generative models to refine molecular hypotheses (Analyse). This feedback loop accelerates optimization, supports multitarget profiling, and enables dynamic model retraining across discovery campaigns.

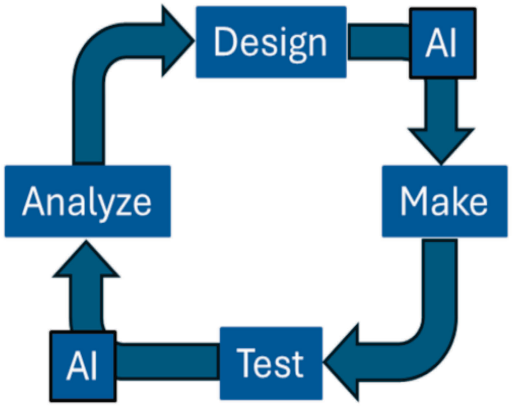

Figure 2. The AI-Enabled DMTA Cycle.

AI also demands interdisciplinary collaboration. Chemists, biologists, data scientists, and software engineers work together in tight loops. Decision-making becomes hypothesis-driven, data-rich, and transparent. This transformation requires all stakeholders, including CROs, to move beyond compartmentalized thinking and adopt a systems-level approach to discovery. The result is not only faster timelines but also smarter discovery: fewer dead ends, more targeted experimentation, and a higher chance of success at the clinic.[1,4,26]

CROs must now decide whether to embrace the future or risk becoming obsolete. The shift to AI-driven discovery necessitates new skills, infrastructure, and approaches to work. First, CROs need to modernize their data infrastructure. Machine learning models require structured, interoperable, and high-quality data. Many CROs are still reliant on spreadsheets and PDFs. The most advanced are investing in electronic lab notebooks (ELNs), laboratory information management systems (LIMS), cloud platforms, and automated data annotation systems. Second, CROs must build or acquire computational capabilities. Some have launched internal AI units. Others have partnered with AI biotech or software vendors. These partnerships often involve data sharing, co-model development, or joint intellectual property (IP) ownership, moving CROs beyond fee-for-service into value creation.[10] Evotec's joint work with Exscientia and Selvita's development of the Target Aware Drug Activity Model (TADAM), for instance, demonstrate how CROs can co-innovate with AI-native companies. [5,27] Figure 3 outlines the primary functional domains where CROs enable and support AI-driven drug discovery. The diagram illustrates the core functional roles that CROs play in supporting AI-driven drug discovery.

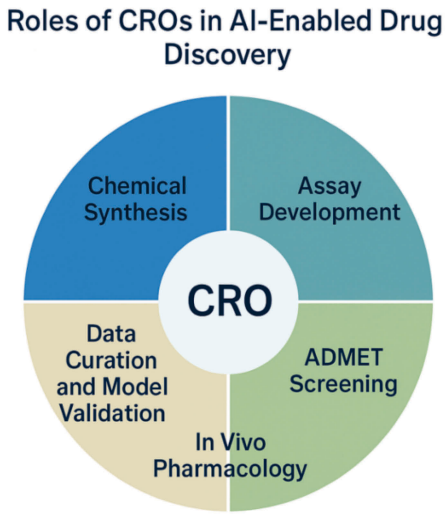

Figure 3. Roles of CROs in AI-Enabled Drug Discovery.

These roles include chemical synthesis, assay development, ADMET screening, in vivo pharmacology, data curation, and model validation. As the AI–CRO interface deepens, CROs must contribute not only experimental data but also structured, model-ready datasets and insights to close the loop between machine learning predictions and laboratory confirmation.[28] Symbolic AI approaches have also proven effective in retrosynthetic planning, where deep learning models are coupled with rule-based systems to generate feasible synthetic routes.[29]

Third, CROs must rethink their service model. Agile, modular, and customizable offerings are now preferred. Clients want to run multiple DMTA loops in parallel and expect CROs to keep pace. CROs like Charles River, Sygnature Discovery, and Aragen are responding by integrating informatics tools and automation into daily workflows.[30–32] Finally, CROs must attract and retain interdisciplinary talent. Scientists who can speak both biology and machine learning are in short supply. Upskilling internal teams is essential. Some CROs have begun offering internal fellowships, data science academies, or cross-functional innovation hubs. Those who adapt will become indispensable innovation partners. Those who do not may be left behind.

The transition to AI-driven discovery is not without challenges. Data quality remains a critical issue. AI systems are highly sensitive to noisy, incomplete, or biased datasets.[33] Many CROs still lack standardized formats, version control, or centralized metadata frameworks, which undermines model performance and slows decision-making. Technological integration is another barrier. AI platforms must connect seamlessly with experimental workflows. This requires investment in digital infrastructure, including interoperable LIMS, cloud-based ELNs, and secure APIs that allow real-time data exchange between clients and CROs. [34,35] Few traditional CROs have these tools in place. Culturally, CROs must shift toward a model of continuous, hypothesis-driven experimentation. This means being flexible with scopes and timelines, allowing for agile workflows, and participating in co-decision making. In short, CROs must evolve from executors to collaborators. However, the upside is significant. CROs that adapt can move up the value chain—becoming co-developers of IP, curators of proprietary datasets, and even licensors of internally developed AI tools. Several CROs are now monetizing their internal AI infrastructure by offering platform-as-a-service models or hybrid discovery partnerships.[36–38]

Table 2. Capabilities Required of Modern CROs.

CAPABILITY	TRADITIONAL CRO	AI-READY CRO
ELN / LIMS Integration	Optional	Mandatory
Computational Expertise	Low	High
Real-time Data Feedback	Rare	Common
AI Partnership Models	Transactional	Collaborative
Model Explainability Support	Not Required	Essential

Internally, AI can improve operational efficiency. Predictive tools can forecast reagent needs, optimize compound logistics, or flag quality control issues in real time. One study showed that AI deployment in a CRO reduced analytical cycle times by 40%.[39] A comparison of traditional and AI-ready CRO capabilities is provided in Table 2. The table compares the typical attributes of traditional CROs with the evolving requirements of AI-ready CROs. While traditional CROs focus on discrete experimental services with minimal digital infrastructure, AI-enabled CROs are expected to support integrated data workflows, contribute to algorithm refinement, and participate in collaborative innovation models. Key differentiators include real-time data sharing, computational expertise, and model explainability support, factors that are essential in modern drug discovery programs driven by artificial intelligence.

Ultimately, AI presents CROs with a unique opportunity: to transition from service providers to strategic discovery engines.

Case Studies

Several CROs have already demonstrated the potential of AI-driven transformation. Table 3 provides a structured overview of how CROs are engaged across different AI-driven discovery applications. It is summarised how typical AI applications are across the drug discovery value chain and the corresponding roles of CROs. It highlights how CROs provide experimental, computational, and data infrastructure to support workflows ranging from target identification to lead optimization. The examples illustrate the diversity of AI models (e.g., graph neural networks, VAEs, reinforcement learning) and the collaborative potential between AI-native biotech companies and CROs.

Evotec, one of the earliest adopters, partnered with Exscientia to bring the AI-designed DSP-1181 to Phase I trials. Evotec provided medicinal chemistry, Drug Metabolism and Pharmacokinetic (DMPK), and safety services that validated AI predictions rapidly and cost-effectively.[41,42] Insilico Medicine took a different approach by developing a fully integrated AI platform spanning target discovery, molecule generation, and clinical trial design. Its fibrosis candidate, INS018_055, progressed from hit to Phase I in just 30 months, less than half the industry average, with support from CROs in China and New Zealand, who handled wet-lab validation and trial management. The seamless integration of deep learning

Table 3. AI-Driven Use Cases and CRO Engagement Models.

USE CASE	AI APPLICATION	CRO ROLE	COMPANIES
Target Identification	Graph-based modeling, NLP mining	Data curation, validation assays	BenevolentAI, BioSymetrics
Target Identification	Graph-based modeling, NLP mining	Data curation, validation assays	BenevolentAI, BioSymetrics
ADMET Prediction	QSAR, ML/Deep Learning	In vitro testing, PK/PD modeling	Atomwise, Cyclica
Phenotypic Screening	High-content analysis, deep learning	Assay development, image analysis	Recursion, Selvita
Lead Optimization	Reinforcement learning, docking prediction	SAR campaigns, analog synthesis	Relay Therapeutics, PostEra

models with high-throughput synthesis and screening workflows enabled this rapid progression. Notably, Insilico's platform also incorporates predictive toxicology and biomarker discovery modules, further accelerating preclinical evaluation and de-risking early development.[43–45]

BenevolentAI advanced BEN-8744 into clinical trials by applying AI to identify a novel target (PDE10) and design selective inhibitors. CRO partners handled synthesis, profiling, and preclinical safety studies. Their responsiveness and data quality were essential to maintaining AI feedback loops. The company's in-house knowledge graph and machine learning platform enabled rapid hypothesis generation and compound prioritization. At the same time, CROs provided the experimental throughput and turnaround times needed to refine the candidate series based on biological feedback iteratively. signals. IR spectra were recorded on an Agilent Cary 630 FTIR instrument. This collaborative model allowed BenevolentAI to progress from target discovery to clinical entry within an accelerated timeframe. Importantly, the integration of AI outputs with real-world CRO workflows demonstrated how distributed teams can co-develop clinical assets when aligned around data standards and shared timelines.[9,46]

Selvita, has expanded its AI capabilities through both internal innovation and strategic partnerships. It developed TADAM, a proprietary tool for data-driven compound selection designed to improve the efficiency of hit prioritization and library design. In collaboration with Ardigen, Selvita also launched High-Content Screening Artificial Intelligence (HiScAI), an AI-powered phenotypic screening platform that integrates high-content imaging with machine learning to predict compound effects. Furthermore, Selvita has licensed the Chemical Protein Stability Assay (CPSA) from Medicines Discovery Catapult (MDC), a UK-based R&D centre. CPSA is a mass spectrometry–based technique for target engagement profiling in lysates, allowing for rapid and label-free assessment of compound binding. By incorporating CPSA into its discovery workflows, Selvita enhances the ability to confirm in vitro target interactions in a high-throughput format.This assay complements Selvita's AI platforms by enabling experimental confirmation of predicted compound–target interactions, thus closing the loop between in silico modeling and biological validation.[27,47,48]

Charles River Laboratories, Sygnature Discovery, WuXi AppTec, and Aragen have also made significant progress. Some CROs have established dedicated data science and cheminformatics groups and are embedding AI into project workflows, particularly in hit triaging, metabolite prediction, and bioassay optimization. For instance, Charles River has developed in-house predictive ADMET models and offers machine learning–enabled lead optimization services. Sygnature Discovery has invested in automated screening platforms and AI-assisted compound profiling to accelerate DMTA cycles. WuXi AppTec is integrating AI tools across its discovery and development services, including AI-driven target identification and digital pathology. Aragen, similarly, has introduced algorithmic decision-making in its assay development pipelines and collaborates with clients to train custom models using proprietary datasets. These initiatives not only enhance internal efficiency but also create new opportunities for clients to participate in more adaptive and data-driven discovery programs.[30–32,49,50] In parallel, the integration of chromatographically derived Experimental Polar Surface Area (EPSA) data, especially from Supercritical Fluid Chromatography (SFC) based methods, into AI models is enhancing the prediction of permeability and passive absorption, improving compound triaging during early screening.[51] CROs such as Selvita are already implementing this approach, developing a combination of high-throughput EPSA profiling with machine learning tools to prioritize compounds for progression better. These initiatives not only enhance internal efficiency but also create new opportunities for clients to participate in more adaptive and data-driven discovery programs. These examples highlight that AI-enabledment is not limited to large pharma – it is achievable, scalable, and already delivering value in diverse CRO contexts.

CONCLUSION

CROs that adapt to AI are poised to evolve into hybrid organizations: part laboratory, part data company, and part innovation partner. This transformation is likely to accelerate over the next decade, driven by both client demand and internal pressures to remain competitive.

One major shift will be the modularization of services. Rather than offering rigid packages, AI-ready CROs will provide on-demand, interoperable services, DMTA cycles in plug-and-play formats that feed directly into client machine learning pipelines. Data will no longer be delivered as static reports but streamed into client dashboards via secure APIs and real-time platforms.

A second shift is IP participation. Some CROs may take equity stakes in early-stage AI biotech, or co-own discovery platforms and compound libraries generated through collaborative models. This is already happening: companies like Evotec and Sygnature have begun co-development agreements in which experimental and algorithmic contributions are jointly protected.

A third area of change will be the internal adoption of AI. CROs that utilize AI not only in client-facing projects but also in operational workflows, such as managing compound logistics, optimizing instrument usage, or anticipating quality control (QC) failures, will benefit from significant efficiency gains. Finally, CROs may increasingly serve as validators of AI claims. As the number of AI-native startups grows, the need for rigorous experimental confirmation becomes even more important. CROs will serve as the proving ground for novel algorithms, helping to differentiate hype from genuine innovation.

In this future, success will not depend solely on scale or cost-effectiveness, but on adaptability, technological fluency, and the ability to collaborate in new, agile ways. AI is no longer a futuristic concept in drug discovery. It is a practical, operational reality reshaping the path from code to clinic. From the emergence of the first AI-designed candidates, such as DSP-1181 and INS018_055, to the widespread adoption of machine learning across the DMTA cycle, the pharmaceutical R&D landscape is undergoing a profound transformation. Figure 4 shows a representative scaffold of DSP-1181, a long-acting 5-HT1A receptor agonist, and a representative PDE10 inhibitor scaffold related to BEN-8744, which was advanced by BenevolentAI into clinical testing for ulcerative colitis following AI-driven target identification and optimization. Structures shown are illustrative and based on publicly disclosed analogues or pharmacophores associated with the respective drug classes.

Contract Research Organizations, once relegated to tactical roles in synthesis or screening, are now positioned at the epicentre of this shift. Symbolic AI approaches have also proven effective in retrosynthetic planning, where deep learning models are combined with rule-based systems to generate feasible synthetic routes. To remain relevant, CROs must do more than keep pace. They must lead in digital integration, invest in data and automation infrastructure, form strategic AI partnerships, and embrace flexible, interdisciplinary modes of collaboration. The case studies presented, from Evotec's partnership with Exscientia to Selvita's in-house development of AI-enabled tools like TADAM and HiScAI, demonstrate that CROs of all sizes can seize this opportunity. Those that rise to the challenge will not merely survive in the AI era; they will help define it.

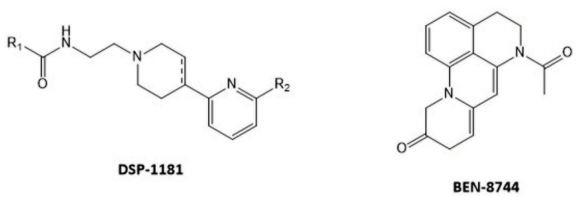

Figure 4. Representative Structures of AI-Designed Clinical Candidates.

As pharmaceutical discovery becomes more iterative, data-driven, and AI-assisted, the CROs that adapt will become indispensable partners in innovation, facilitating a new kind of discovery ecosystem where experimentation, prediction, and validation are inseparable. Despite the breakthroughs, scepticism remains regarding overpromising and underdelivering. Ensuring reproducibility, interpretability, and regulatory alignment is crucial for sustainable impact.

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