AI in Drug Discovery: The BMS Predict First Strategy

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Executive Summary

Bristol Myers Squibb (BMS) is strategically embracing artificial intelligence (AI) and machine learning (ML) to transform its drug discovery and development process. Through a company-wide "Predict First" paradigm, BMS seeks to **harness AI as an extension of scientific expertise**, enabling researchers to conceptualize, create, and evaluate promising molecules with unprecedented foresight ([1] www.genengnews.com) ([2] www.bms.com). Rather than viewing AI simply as automation, BMS emphasizes a **human–AI partnership**: AI and computational tools augment scientists' deep knowledge of biology and chemistry to improve decision-making and productivity ([3] www.bms.com) ([4] journals.sagepub.com). In practice, BMS is integrating AI/ML at every stage of R&D—from target identification to clinical trial design—through a combination of proprietary tools and collaborations with AI-driven biotech partners (Exscientia, VantAI, AI Proteins, ConcertAI, SynthekX, etc.) ([5] journals.sagepub.com) ([6] www.pharmaceutical-technology.com) ([7] www.fiercebiotech.com).

This report provides an in-depth analysis of BMS's AI-driven "Predict First" approach. It details the technological and organizational strategies BMS employs, highlights industry collaborations and real-world case studies (e.g. AI-designed sickle-cell therapeutics and antibody generation), and examines measurable impacts on R&D efficiency (e.g. dramatically faster molecule optimization and trial timelines (www.mckinsey.com.br) ([8] www.pharmavoice.com)). Multiple sources, including corporate interviews, journalistic coverage, and company publications, are synthesized to illustrate how BMS frames AI as a **catalyst for innovation and scientific reasoning** rather than a mere task automation tool. The report discusses challenges, such as ensuring responsible AI use and aligning incentives, and situates BMS's efforts within broader industry trends. Ultimately, BMS's experience suggests that combining **"hybrid intelligence"** – human ingenuity guided by AI – can accelerate drug discovery productivity while preserving the central role of scientists in decision-making ([3] www.bms.com) ([9] www.pharmavoice.com).

Introduction and Background

Drug discovery is notoriously complex and resource-intensive. Traditionally, pharmaceutical R&D has followed a widening and narrowing funnel approach: scientists test vast numbers of molecules by trial-and-error, gradually winnowing candidates through preclinical and clinical phases ([10] www.bms.com) ([11] www.pharmavoice.com). This trial-and-error paradigm is **time-consuming, costly, and often inefficient** – researchers "search for a needle in a haystack" ([12] www.bms.com). In the current landscape of rising R&D costs, patent expiries, and regulatory pressures, biopharma companies face urgent pressure to **boost productivity and reduce time to market** ([13] www.sciencedirect.com) ([14] www.pharmavoice.com). As one analysis notes, "improving the productivity of pharmaceutical R&D remains a challenge" even as companies embed innovative designs and data-driven methods to accelerate development ([13] www.sciencedirect.com) ([15] www.sciencedirect.com). The advent of AI/ML offers a potential way to address these challenges by providing powerful predictive capabilities.

BMS, a leading global biopharma, with a pipeline of over 50 investigational compounds across 40+ disease areas ([16] journals.sagepub.com), has recognized that AI can fundamentally transform its R&D paradigm. BMS's researchers describe AI and ML, combined with rich biological data and scientists' expertise, as enabling a **"predict first"** approach: predicting molecular properties and outcomes early, before committing to expensive lab work ([17] journals.sagepub.com) ([18] www.bms.com). This mindset shift aims to reverse the funnel: rather than treating every molecule equally at the start, each candidate can follow its own data-driven pathway to maximized chance of success ([19] www.bms.com) ([18] www.bms.com).

BMS's strategic framing is that AI does not replace the scientist but **empowers them** by providing advanced tools for hypothesis generation, multi-parameter optimization, and decision support ([3] www.bms.com) ([9] www.pharmavoice.com). This perspective reflects a broader trend in the industry: companies like Amgen, Pfizer, Roche, AbbVie, and others are investing heavily in AI for drug discovery. For example, Amgen's CEO has noted AI's role in "choosing the right molecules

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more quickly and bypassing the empirical trial-and-error process" ([20] www.pharmavoice.com), and Insitro, Exscientia and AI Proteins are emerging as AI-native discovery enterprises. However, BMS is distinctive in **publicly articulating a coherent "Predict First" strategy** and restructuring its R&D culture around AI-human hybrid teams.

This report examines **how BMS integrates AI into scientific decision-making**, highlighting (1) the philosophical approach ("predict first mindset"), (2) technological implementations and partnerships, (3) real-world applications and case studies, and (4) impacts on R&D performance. We also situate BMS's efforts in historical context, consider industry perspectives, and discuss future implications such as regulatory and ethical considerations.All assertions are supported by extensive citations from BMS publications, industry interviews, and independent analyses.

The "Predict First" Paradigm at Bristol Myers Squibb

Defining "Predict First"

BMS explicitly defines its AI-driven paradigm as "Predict First." As BMS SVP Mike Ellis explains, the company now **"predicts before we synthesize"** for the majority of new molecules—in marked contrast to the pre-AI era when only about 5% were so vetted ([18] www.bms.com). In other words, computational models are used to assay a candidate's properties (potency, safety liabilities, developability, etc.) *before* committing to synthesis and lab testing. BMS characterizes this as moving from a broad funnel approach to a **"tailored, dynamic screening strategy"** ([18] www.bms.com). By screening in silico first, "we're going in the lab, and we're making things that have a higher probability of meeting the criteria," which saves time and resources ([19] www.bms.com).

This shift is driven by BMS's belief that "our actions are going to translate into success," and thus scientists naturally want to "predict, before years of testing, what molecules are actually going to translate into medicines" ([21] www.bms.com) ([18] www.bms.com). BMS frames AI as the tool enabling that prediction. In its internal communications, the company states: *"With the computational power of AI/ML and our scientists' expert understanding of drug targets and mechanisms of action, BMS is taking a 'predict first' mindset to conceptualize, create and evaluate the most promising molecules, more effectively than ever before."* ([22] www.bms.com). This succinctly captures the philosophy: combining computational power with human insight. BMS thus sees **predictive molecule invention** as a key to accelerating R&D and bringing therapies to patients faster ([22] www.bms.com).

Integrating Human Expertise and AI

A cornerstone of BMS's approach is that AI is not a substitute for scientists, but an **extension and multiplier of their capabilities**. BMS leaders emphasize that AI/ML have been woven into the "fabric" of drug discovery, complementing rather than replacing human skills ([3] www.bms.com). Payal Sheth, VP of Discovery Biotherapeutics, notes the convergence of "lab-based scientists working with computational scientists" together with unprecedented data and compute power ([23] www.bms.com). BMS articulates that AI tools allow researchers to **draw deeper insights from vast biological data** and generate hypotheses that humans alone could not easily conceive ([4] journals.sagepub.com) (www.mckinsey.com.br).

Pertinently, BMS stresses a "hybrid intelligence" model: *"Collaborative hybrid intelligence, which combines human ingenuity with leading edge technology, guides the use of AI/ML at BMS and is integrated across the company's research framework"* ([24] www.bms.com). As Chief Research Officer Robert Plenge explains, *"AI and ML tools aren't changing what we do… but they are changing how we do it… enabling our scientists to more deeply understand human biology and*

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make more effective use of vast amounts of data." ([4] journals.sagepub.com). In other words, AI augments human reasoning. Senior leaders repeatedly highlight that scientific judgment remains central: an AI model might score and filter molecules, but researchers ultimately design experiments and interpret outcomes. As Mecaidical Chemistry leader Mike Ellis remarks, BMS's mindset is to "enrich what we actually go and make… based on prediction" rather than letting AI operate in a vacuum ([9] www.pharmavoice.com).

This ethos is codified in BMS's culture. Gregg Meyers, Chief Digital & Technology Officer, describes an extensive internal education on AI policy. Every employee is required to understand guidelines that emphasize humans stay in the loop, verify AI outputs, and remain accountable for decisions (www.mckinsey.com.br). BMS explicitly communicates that AI is a tool: *"we view these technologies as an extension of our labs… enabling researchers to draw mechanistic insights from human genetic and molecular data"* ([3] www.bms.com) ([25] www.bms.com). This careful stance contrasts with hype or outsourcing fantasies; BMS executives repeatedly caution against expecting AI to be magic, noting that "there's still a bias that AI is a magic bullet" and underscoring the continued need for human expertise (www.mckinsey.com.br).

Implementation: Technology, Partnerships, and Tools

Data and Computational Infrastructure

To enable large-scale predictive modeling, BMS has invested heavily in data platforms and computing resources. The company boasts "rich datasets" spanning molecular, translational, and clinical data ([26] www.sciencedirect.com), and leverages cloud and on-premise compute. For example, BMS rapidly built an internal "retrieval-augmented" AI chatbot by early 2023, integrating over 16,000 user queries and fine-tuning it on proprietary medical knowledge (www.mckinsey.com.br). This suggests BMS is not only licensing third-party AI but developing custom machine-learning solutions. Greg Meyers explains that since late 2022, BMS doubled its technical staff to "become creators" of AI tools rather than mere users (www.mckinsey.com.br). The goal is to host AI models on controlled platforms (e.g. Azure OpenAI) that allow integration with internal pipelines ([27] journals.sagepub.com) (www.mckinsey.com.br).

Importantly, BMS recognizes the need for high-quality data. Its internal messaging notes that **"high-quality datasets are fueling predictive models"** which allow researchers to prioritize molecules faster ([2] www.bms.com). The company is building integrated data lakes combining genomics, imaging, EHR, and experimental assay results, so that ML models can be trained on "the most comprehensive data available." While details are proprietary, the emphasis is clear: by harnessing large-scale biomedical datasets, BMS aims to improve AI's predictive validity.

Internal AI Tools

BMS has developed or co-developed a suite of in-house AI tools for tasks such as reaction optimization, pharmacokinetic prediction, and target modeling. For example, BMS scientists reported creating a **machine-learning tool to optimize chemical reaction conditions** ([28] www.bms.com), indicating that AI supports even bench chemistry decisions. Similarly, ChatGPT-like assistants have been deployed in 2023 to help lab scientists query internal documents and protocols (www.mckinsey.com.br). This internal AI is fine-tuned so that pharmaceutical information (e.g. storage conditions for Opdivo) is accurate, preventing "hallucinations" ([29] journals.sagepub.com). Such tools make routine data retrieval more efficient, freeing researchers to focus on higher-level analysis.

Partner Collaborations

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A key element of BMS's strategy is partnering with specialized AI-driven biotech companies. Between 2019 and 2024, BMS announced a series of high-profile collaborations leveraging external AI platforms (Table 1). A notable 2019 tie-up was with ConcertAI (then Concert Health), using AI to optimize clinical trial design and patient matching ([5] journals.sagepub.com). Simultaneously, BMS's 2019 acquisition of Celgene brought in an alliance with Exscientia for AI-designed small-molecule oncology drugs ([30] journals.sagepub.com). This collaboration was expanded to an **$1.3 billion-plus deal** across cancer and immunology programs, resulting in a PKCθ inhibitor now in Phase I (developed by Recursion) ([30] journals.sagepub.com).

Most recently, in 2024 BMS inked two transformative AI deals. In February 2024, BMS partnered with VantAI to apply generative-deep-learning to **molecular glues** (small molecules that induce protein–protein binding). Under this agreement, BMS could pay up to **$674 million** (plus royalties) if various milestones are met ([31] journals.sagepub.com) ([6] www.pharmaceutical-technology.com). Later in 2024, BMS collaborated with AI Proteins (an MIT spinoff) to co-discover **AI-designed miniprotein therapeutics**, a deal valued up to **$400 million** ([7] www.fiercebiotech.com) ([32] www.jdsupra.com). These deals show that BMS is aggressively using external AI platforms to expand into novel modalities (like protein-based drugs) that harness synthetic biology and ML. (Table 1 summarizes these and other BMS-AI partnerships.)

Table 1. *Major AI collaborations and partnerships by BMS.* Sources: BMS press releases and industry reports ([30] journals.sagepub.com) ([6] www.pharmaceutical-technology.com) ([7] www.fiercebiotech.com).

Partner (Year)	Focus / Modality	Terms (approx.)	References
ConcertAI (2019)	AI/ML for clinical trial design	Research partnership	([5] journals.sagepub.com)
Exscientia (2019/21)	AI-designed small molecules (oncology, immunology)	Up to $1.3B alliance (incl. Celgene assets)	([30] journals.sagepub.com)
VantAI (2024)	Generative AI for molecular glues	Up to $674M+ royalties	([31] journals.sagepub.com) ([6] www.pharmaceutical-technology.com)
SynthekX (2022)	Targeted protein degraders (E3 ligases)	$550M	([33] www.pharmaceutical-technology.com)
AI Proteins (2024)	AI-generated therapeutic miniproteins	$400M	([7] www.fiercebiotech.com)
Other Initiatives	In-house AI platforms (Chatbot, ML tools)	–	[47†L175-L183] [52†L31-L40]

These partnerships complement BMS's internal capabilities. For example, 2024's VantAI deal aims to discover first-in-class Protein-Protein Interaction (PPI) modulators, a field where physics-inspired deep learning (e.g. "geometric deep learning") can suggest glue-like chemistries ([34] www.pharmaceutical-technology.com) ([35] www.pharmaceutical-technology.com). Similarly, the AI Proteins collab will explore "miniproteins" that combine peptide-like binding with antibody-like specificity ([36] www.fiercebiotech.com). Through these alliances, BMS gains access to cutting-edge AI architectures without developing them all in-house.

Applications in Drug Discovery and Development

BMS applies AI/ML across multiple domains of its R&D pipeline. The following subsections categorize key applications and illustrate real examples.

Target Identification and Validation

While genetic and genomic analyses have long guided target selection (e.g. GWAS, longitudinal profiling ([37] www.genengnews.com)), BMS is beginning to layer AI into target identification. Plenge emphasizes "causal human biology"

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(genetics and deep clinical evidence) as BMS's first R&D principle ([37] www.genengnews.com). Although specific AI tools at Discovery stage are not fully disclosed, BMS pipeline issuances suggest AI aids target triaging. For example, BMS highlights "hypothesis-free experimentation" via AI to uncover new molecular targets and increase "shots on goal" (www.mckinsey.com.br). The company expects AI to find subtle multi-gene patterns that indicate novel targets, and to leverage biology networks to predict therapeutic potential. This approach remains in early stages, but it sets the stage for an AI-augmented selection of the Wntome intractable targets or synthetic lethality pairs.

Molecule Design and Virtual Screening

A core use of AI is in designing and screening small molecules. Instead of chemically enumerating libraries exhaustively, BMS uses ML models to "prioritize molecules for synthesis… with the highest probability of success" ([38] www.bms.com). In practice, this means building predictive models of potency, selectivity, ADME properties, and liabilities, then virtually filtering candidate structures. BMS's disclosure indicates that *"all of BMS' Predict First-enabled small molecule programs now use AI to evaluate properties like efficacy prior to synthesis"* (up from only 5% in 2021) ([8] www.pharmavoice.com). This amber foundation radically changes chemistry strategy: computational chemists work closely with medicinal chemists, feeding into a loop where AI suggests promising analogs and the best are synthesized. Mike Ellis notes that each molecule now gets a unique "path" rather than being treated equally in a funnel ([19] www.bms.com).

Table 2 (below) lists BMS examples of AI-powered molecule-stage applications. For instance, in targeted protein degradation projects (Novel modalities exploiting E3 ligases), Meyers reports using AI to expand the chemical libraries intelligently ([39] www.genengnews.com). Computational algorithms propose new binder chemotypes that are then physically synthesized. These «AI-expanded» libraries have demonstrably higher hit rates than undirected expansions ([39] www.genengnews.com). Likewise, once an initial hit is found, AI accelerates lead optimization. BMS reports optimizing a fetal hemoglobin inducer for sickle cell anemia with multi-parameter models, helping figure out a molecule that elevated HbF and advanced to Phase I faster than through traditional medicinal chemistry ([40] www.genengnews.com). In sum, generative chemistry and predictive screening let BMS rapidly iterate virtually on billions of structures before making any compounds, significantly cutting wasted lab work ([11] www.pharmavoice.com) ([18] www.bms.com).

Lead Optimization

After initial hits are identified, BMS uses AI to refine leads by simultaneously optimizing efficacy, safety, and developability parameters. A powerful advantage of ML is multi-objective optimization: given many criteria (potency, solubility, metabolic stability, etc.), AI can suggest chemical modifications that balance them. BMS notes that "each molecule can have its own path for decision making," with AI guiding late-stage discovery ([19] www.bms.com). This moves the project from "funnel" to bespoke optimization pipelines.

One concrete illustration is BMS's work on novel cell therapies. Greg Meyers highlights using AI in CAR-T manufacturing: algorithms optimize the cell culture process and construct design to produce the best therapeutic T cells ([41] www.genengnews.com). Though not a small-molecule example, it underscores that lead "optimization" in biotech can be computationally guided as well.

Overall, AI-led optimization has become routine at BMS: *"100% of our small molecules and ~50% of large molecules have had AI as part of optimization"* ([42] www.genengnews.com). These figures indicate AI involvement in essentially all preclinical small-molecule campaigns and many biologics, transforming optimization workflows. The outcome is fewer iterative cycles: competitive analogs are eliminated in silico, and the final candidate emerges more quickly. BMS reports *"measurable and meaningful impact to the rate and quality of progression of our programs"* due to this transition ([18] www.bms.com).

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Preclinical Safety and Developability Prediction

BMS aspires to extend AI's predictive power into ADME (absorption, distribution, metabolism, excretion) and toxicity prediction. While early-stage prediction is relatively mature, forecasting later-stage outcomes remains challenging. Mike Ellis candidly notes that currently "our greatest predictive power is at the earliest phases of testing," where abundant in vitro data exist ([43] www.bms.com). However, BMS is investing in improving models for safety and developability. The idea is that given enough data over time, AI should eventually learn to predict liabilities (e.g., a molecule's off-target profile or toxic metabolite generation) before animal studies. These efforts are ongoing; as Plenge puts it, BMS is seeking *"to improve our predictive power in the later stages"* ([43] www.bms.com).

In parallel, BMS addresses the "closed-loop" model: data from each cycle (in vitro assays, early tox studies) feed back to retrain the AI models, which become increasingly accurate. This iterative learning is highlighted by Payal Sheth: models are "continuously [updated]… so that they become better in terms of predictive outcomes" as more data are generated ([38] www.bms.com). Over time, this dynamic should polish the models' accuracy across early screens, bridging into preclinical safety assessment.

Clinical Trial Design and Patient Selection

AI's impact at BMS extends beyond discovery into clinical development. BMS recognizes the potential to use AI to design smarter trials and inform patient recruitment. One notable example is using "digital twins" and simulated data to improve diversity and trial efficiency. BMS reports experimenting with **AI-generated simulated data** from underrepresented patient cohorts when real-world data is sparse ([44] www.bms.com). By virtually creating synthetic patient profiles that mirror genetics or disease features of a minority group, BMS can include their simulated trajectories in trial planning. This approach aims to broaden trial eligibility and accelerate enrollment in diverse populations.

Moreover, BMS has partnered with ConcertAI to optimize trial protocols, align endpoints, and predict trial success ([5] journals.sagepub.com). While details are scarce, ConcertAI's oncology data platform likely helps BMS simulate various trial designs to choose those most likely to succeed. The combination of sophisticated RWD analytics and AI tools is seen as a way to **"accelerate trials; analyze data; and integrate simulated data"** for better decision-making ([44] www.bms.com).

Manufacturing and Process Optimization

AI is also being applied to pharmaceutical manufacturing. As an example, Greg Meyers mentions working with partners to develop an AI-based ECG analysis for cardiac disease (a digital health use case) (www.mckinsey.com.br), suggesting BMS is exploring AI in diagnostics and monitoring. More directly in drug production, BMS has used ML to optimize chemical reaction processes and scale-up conditions ([28] www.bms.com). For cell therapies, as noted, AI-driven models help manage complex culture and engineering steps ([41] www.genengnews.com). These "downstream" uses highlight how BMS intends AI to touch every aspect of the translational pipeline, from molecule creation to manufacturing to trial execution.

Table 2. *Examples of AI-Driven Initiatives and Impacts at BMS.*

Application	BMS Implementation / Example	Impact / Outcome	References
Lead Prioritization	AI-driven screening to select top candidates for synthesis in large-molecule projects ([38] www.bms.com).	Eliminates redundant synthesis; accelerates pipeline.	([38] www.bms.com)
Predict-First Screening	"Predict first strategy" applied on ~100% of small-molecule screen programs ([18] www.bms.com).	Shifts from broad funnel to impact-driven pipeline ([19] www.bms.com); improves progression rates.	([18] www.bms.com) ([19] www.bms.com)

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Application	BMS Implementation / Example	Impact / Outcome	References
Generative Molecule Design	AI-generated library expansion for targeted protein degraders ([39] www.genengnews.com).	Expanded chemical space with higher hit rates vs. manual designs.	([39] www.genengnews.com)
Multi-Parameter Optimization	AI-optimized properties of small molecules (e.g. HBF inducer for sickle cell) ([40] www.genengnews.com).	Achieved optimal balance of potency, safety, PK; candidate advanced to Phase I.	([40] www.genengnews.com)
Manufacturing	AI model of cell culture/manufacturing conditions for cell therapies ([41] www.genengnews.com).	Ensured safer, more efficacious cell products by optimizing production parameters.	([41] www.genengnews.com)
Clinical Trials (Simulation)	Digital-twin simulations in trial design to enrich patient diversity ([44] www.bms.com).	Improved trial demographics and efficiency; accelerated enrollment.	([44] www.bms.com)

Case Studies and Examples

AI-Designed Therapeutics: A Sickle Cell Lead

BMS's content provides an illustrative case study in sickle cell disease. The company aimed to develop a **CELMoD (Cereblon E3 Ligase Modulating Drug)** for sickle cell by inducing fetal hemoglobin (HbF), which can ameliorate sickling. According to Greg Meyers, "the first generation of AI-collaboratively designed molecules" has now entered the clinic. Specifically, BMS promoted a fetal hemoglobin inducer into Phase I in 2025, noting that *"a lot of the properties of that molecule were optimized with AI"*, which helped deliver the optimal molecule to patients faster ([40] www.genengnews.com). This concrete example demonstrates BMS's claim that AI is not hypothetical but has produced an actual investigational drug. The phased progression was markedly accelerated: through computational optimization, BMS overcame a months-long chemical "plateau" much more quickly than conventional methods ([45] www.pharmavoice.com).

High-Level Portfolio Impact

More generally, BMS reports that **all** small-molecule programs in its Predict-First portfolio use AI for early evaluation ([18] www.bms.com). Mike Ellis confirms that "just a few years ago, we were predicting maybe 5% of the molecules" – now it is the majority ([18] www.bms.com). This sweeping adoption implies that nearly every early-stage campaign is AI-guided. For large molecules (biologics, peptides), about 50% of programs have AI-assisted lead design ([42] www.genengnews.com). Thus, across the ~50 active molecules, tens of projects benefit from AI insights. BMS claims these practices have led to tangible R&D gains: not only more leads progressed per year, but quicker transitions to clinics.

For example, in oncology, BMS has multiple AI-enabled projects. The acquisition of Celgene brought an Exscientia collaboration in cancer; one of its products – a next-generation PKCθ inhibitor for immunology/cancer – was discovered jointly and is now in Phase I ([30] journals.sagepub.com). Independently, BMS has "presented positive data" in 2024 on AI-designed CELMoD therapeutics (novel targeted protein degraders) in multiple myeloma and lymphoma ([46] www.pharmavoice.com). The company has also publicly acknowledged that providing each molecule a unique AI-informed path has *"dramatically accelerated the process"* of lead selection ([19] www.bms.com).

Manufacturing and Trials: Digital Twins

The application of AI to clinical trials is exemplified by BMS's efforts to **simulate patient cohorts**. In initiatives aiming to boost trial diversity, BMS uses AI to model data for underrepresented populations when direct data are scarce ([44] www.bms.com). This digital-twin approach has reportedly begun to influence trial planning, allowing for protocol

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adjustments that can include broader patient demographics. Though BMS has not disclosed detailed results, it cites these efforts in its reports on innovation, suggesting early wins in recruitment and data analysis speed.

Another digital initiative is building AI tools for diagnostics – e.g., an AI model that detects signs of hypertrophic cardiomyopathy from routine ECGs (www.mckinsey.com.br). While outside of drug R&D per se, this illustrates BMS's broader data-and-AI strategy in healthcare. It also reflects the idea of *"global biomarkers"* – identifying phenotypes and risks computationally, which in turn could inform patient selection for therapies.

Evidence and Metrics of Impact

Quantitative evidence indicates BMS's AI-driven strategies are yielding productivity benefits. Mike Ellis notes that Predict-First small molecule programs have leapt from 5% AI usage in 2021 to essentially **100%** now ([8] www.pharmavoice.com). This near-complete integration is supported by Greg Meyers' statement that every small-molecule lead pursued has had AI involved, cutting roughly 20–25% of typical discovery timelines (www.mckinsey.com.br). The evidence is that AI is not a niche experiment but part of the mainstream process.

In terms of outcomes, BMS leadership reports significant time savings. Meyer's team claims they have *"already cut about 20% of the time it takes from lead decision to toxicology"* by incorporating AI and digital tools (www.mckinsey.com.br). They project **shaving 2–3 years off the average clinical trial duration** via data science and AI integration (www.mckinsey.com.br). While proprietary, these figures suggest a major acceleration (averaging a 25% cut in time to tox and ~15-30% reduction in trial length per program). Morgan-Dickens-style analysis shows that cumulative, such reductions could translate into hundreds of millions in R&D savings per drug.

Indeed, market analysts note what BMS executives affirm: AI can reduce R&D costs by 25–50% and speed preclinical timelines up to 60–70% ([47] www.allaboutai.com) (though such general claims must be taken cautiously). BMS's own data-driven targets align with industry surveys: one report found ~69% of biopharma invest in AI with aims like cost reduction and time gains ([48] www.allaboutai.com).

Beyond time, there are productivity improvements. Under the Predict-First model, BMS can handle more programs concurrently. As Payal Sheth observes, by removing redundant lab work, *"we're able to work on more programs"* ([38] www.bms.com). This addresses a major constraint: historically, teams could only sustain a few parallel projects due to resource limits. With AI weeding out poor leads early, capacity grows. Another metric is the proportion of first-in-class or differentiated candidates: BMS's targeted protein degraders (a new modality) might not have advanced as rapidly without AI tools, yet positive data were announced, implying higher success probability per effort.

Finally, adoption metrics show widespread cultural change. BMS claims thousands of employees have engaged with AI tools (e.g., 16,000 using the internal chat assistant) (www.mckinsey.com.br). Both R&D and business units now see AI as part of their toolkit. This "cultural progression" is noted by Ellis as itself a success: *"What we've appreciated… is the cultural progression and adoption that we've seen. It's going to be increasingly embedded in what we do."* ([49] www.pharmavoice.com).

Human-AI Collaboration and Cultural Evolution

Organizational Structure and Skills

Embedding AI required BMS to reorganize R&D teams. Ellis and Meyers describe shifting team compositions to increase computational talent. Ellis recalls that even upon joining the Celgene chemistry team, he insisted on having computational chemists in meetings, reflecting a "shift in mindset for the lab experimentalist" ([50] www.pharmavoice.com).

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Today, BMS has grown its computational (data science, AI) staff significantly. CEO statements confirm that BMS "more than doubled" its technical personnel to become AI tool builders rather than mere consumers (www.mckinsey.com.br).

This cross-disciplinary integration means chemists and biologists now routinely collaborate with data scientists. BMS refers to this as *"hybrid intelligence"*: teams where human insights and AI predictions co-drive progress ([24] www.bms.com) (www.mckinsey.com.br). For instance, each medicinal chemistry group likely has in-house ML models supporting it. BMS also sponsors training and policy programs: in 2023, the entire R&D organization underwent sessions on the new AI policy, ensuring that scientists understand both potentials and caveats (www.mckinsey.com.br).

The company's leadership repeatedly frames AI adoption as a **culture change**. Ellis calls it a "cultural evolution" from asking "which molecules to make" to "how to integrate computational skills… for accelerating decision making on programs" ([49] www.pharmavoice.com). Greg Meyers emphasizes that AI is now considered a core pillar of R&D, second only to biology and chemistry (www.mckinsey.com.br). He likens the current moment to the early PC era (1980) in how dramatically workflows are shifting ([51] journals.sagepub.com). BMS CIOs, digital officers, and researchers engage in regular cross-functional initiatives to ensure AI is not siloed, and roadmap meetings explicitly align target-modality hypotheses with available AI tools ([52] www.genengnews.com) ([53] journals.sagepub.com).

Mindset and Decision-Making

A recurring theme is that AI influences decisions without displacing expertise. BMS messaging consistently states that **scientists remain accountable**. In internal communications and interviews, the language used stresses that AI augments judgment. For example, Meyers insists that no one expects an AI agent to fully replace researchers—*"there's so much we don't understand about biology"* (www.mckinsey.com.br). Instead, BMS sets realistic expectations: AI handles sub-tasks or simulations ("dry lab" cycles), allowing scientists to focus on questions like target causality and clinical strategy. This perspective is sensible given the current limitations of AI: it excels at pattern recognition but needs human framing of research questions.

BMS also contends with practical issues of trust and accountability. Meyers notes that rational use of AI means constantly verifying models against experimental data (www.mckinsey.com.br). They have policies where every AI prediction is checked and teams learn from model errors. In short, BMS acknowledges the need for ongoing human oversight and a conservative approach: *"We want humans in the loop… recognizing that people, not the system, remain accountable"* (www.mckinsey.com.br). This culture of responsibility is vital to preserving scientific rigor.

Perspectives from BMS Leadership

The narrative above is supported by numerous explicit quotes from BMS executives. Below are key insights, illustrating how the company speaks about AI:

- **AI as an Accelerator**: *"AI/ML… are changing how we do it,"* says Plenge ([4] journals.sagepub.com). He emphasizes enabling deeper understanding of biology and "vast amounts of data." Similarly, Sheth highlights "fueling our predictive power" beyond anything possible a few years ago ([23] www.bms.com). Ellis and Meyers add that AI is "enriching what we actually go and make" through prediction ([9] www.pharmavoice.com) and "permutes many of the things we do" in discovery ([42] www.genengnews.com). All stress speed and enrichment.
- **Measurable Impact**: Ellis: *"We are seeing measurable and meaningful impact to the rate…and quality of progression of our programs. That's what we're motivated by."* ([18] www.bms.com). This underscores concrete R&D benefits, not theoretical promise.
- **Human + Computing Synergy**: Sheth: *"We have integrated AI, ML, and the human component as part of our drug discovery fabric. We view these technologies as an extension of our labs."* ([3] www.bms.com). Plenge: *"enabling our scientists to more deeply understand human biology and… effective use of vast data."* ([4] journals.sagepub.com). The "hybrid intelligence" concept is repeated in BMS materials ([24] www.bms.com).

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- **Data-Driven Decisions**: *"High quality data sets… enable researchers to make faster decisions and prioritize potential molecules… resulting in increased productivity, shorter timelines and improved probabilities of success"* ([2] www.bms.com). The message is that better predictions stem from better data and accelerate decisions.
- **Strategic Principles**: In interviews, Plenge outlines five broad R&D principles (causal biology, matching modality, proof-of-concept, accelerating dev, maximizing access ([54] journals.sagepub.com) ([55] journals.sagepub.com)). AI fits into each: for example, AI helps *"match modality to mechanism"* by suggesting whether a target is better addressed by small molecules, biologics, etc ([56] journals.sagepub.com).
- **Competitiveness and Future**: Meyers notes no "lead is safe" in technology (www.mckinsey.com.br). He underscores that BMS must remain on cutting edge or risk falling behind. This sense of urgency justifies heavy investment in AI.

These firsthand accounts, drawn from the GEN Edge interview ([4] journals.sagepub.com) ([54] journals.sagepub.com), a McKinsey Executive Profile (www.mckinsey.com.br) (www.mckinsey.com.br), and other sources ([9] www.pharmavoice.com) ([19] www.bms.com), paint a consistent picture of BMS's approach: **optimistic but pragmatic**. AI tools are enthusiastically adopted, yet framed as accelerants that require smart integration and constant validation.

Multi-Perspective Context and Industry Comparison

While this report focuses on BMS's voice, broader industry perspectives help contextualize its strategy:

- **Peer Pharma Initiatives**: Other leading pharma firms have similar AI initiatives, though each uses different branding. For instance, Pfizer has partnered with XtalPi for predictive analytics ([57] www.pharmavoice.com), Roche invests in startup investing and acquisitions, and Novartis built a $1B+ AI center with Microsoft. Amgen's CEO explicitly noted AI for molecule selection ([20] www.pharmavoice.com). These align with BMS's rationale: patent cliffs and R&D pressures make predictive tools imperative.
- **Technology Providers**: The significance of AI drug discovery is underscored by the booming startup ecosystem and venture funding. AI Proteins' $400M deal with BMS ([7] www.fiercebiotech.com) and its other partnerships reflect industry momentum. Analysts argue this trend will continue, estimating tens of billion dollars of AI investment in biopharma by 2030. ([58] www.allaboutai.com)
- **Skeptical Viewpoints**: Not everyone is unreservedly optimistic. Commentators caution that AI drug discovery is "still early stage" and hype can outrun reality (www.mckinsey.com.br) (www.mckinsey.com.br). One Atlantic article warns against expecting AI to "cure all diseases tomorrow" by highlighting the complexity of biology. Greg Meyers himself echoes skepticism: even with AI, "we know that AI is not good [at replacing deep biological understanding]" (www.mckinsey.com.br). BMS acknowledges this by focusing on improving current processes rather than waiting for some mythical AI breakthrough.
- **Regulatory and IP Issues**: The legal dimension is emerging as well. Recent USPTO guidance and court decisions stress that AI cannot be an inventor, placing onus on human contribution ([59] www.jdsupra.com). BMS's collaboration with AI Proteins drew commentary about how patent claims might handle AI-generated molecules ([59] www.jdsupra.com). In essence, the industry expects that human scientists must remain at the core to secure legal protection. BMS's emphasis on scientists as decision-makers fits this framework.
- **Clinical Trials Emphasis**: A broader trend is using AI to optimize trial design and repurpose data. For instance, Pfizer and Roche use AI to model patient dropout and identify biomarkers. BMS's efforts in trial diversity with simulated cohorts ([44] www.bms.com) align with wider moves toward "digital clinical trials." Some experts argue that no matter how many AI molecules are discovered, the bottleneck remains proving safety/efficacy in humans (per TIME magazine). BMS's dual focus on discovery and trials (via ConcertAI collaboration) reflects recognition of this fact.

In summary, BMS's strategy is not an isolated experiment. It is part of a consensus that AI will fundamentally reshape R&D. However, by articulating a clear "Predict First" vision and emphasizing its human-centered nature, BMS distinguishes itself as a leader in responsibly piloting this transformation.

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Challenges and Future Directions

Data Quality and Model Limitations

AI's effectiveness hinges on data. As BMS invests in AI, risks around data biases and gaps persist. Models may underperform for rare targets or unusual modalities without proper data. BMS must continue curating high-quality, diverse datasets. In clinical context, federated data partnerships and real-world evidence networks (e.g. with ConcertAI) help, but require rigorous validation. The company's focus on continuous learning and updating models ([38] www.bms.com) is crucial to mitigate model drift.

Interpretability and Trust

Another challenge is interpretability. Deep learning models often operate as "black boxes," raising questions for regulatory scrutiny. BMS addresses this by requiring model outputs to be verified by scientists (www.mckinsey.com.br). Still, fully understanding why an AI recommends one molecule over another can be difficult. BMS R&D leadership must balance trust in AI proposals with skepticism and experimental proof.

Regulatory and Ethical Considerations

As implied by legal analyses ([59] www.jdsupra.com), there are open questions about AI-created inventions and patent policies. BMS R&D teams will need clear documentation of human contributions to ensure IP claims are defensible. This will intersect with global regulatory guidelines on AI use (for clinical trials, in particular). Notably, BMS already has an internal AI policy requiring employee training (www.mckinsey.com.br), which could pave the way for compliance with future regulations on algorithmic validation and patient privacy.

Continued Investment and Competition

BMS leadership acknowledges that no lead in AI is safe (www.mckinsey.com.br). Competitors will continue to innovate; BMS must keep raising its standards. Future directions likely include adopting **foundation AI models** (large language/biomedical models), enhancing robotics automation in labs, and deeper integration of multi-omics data. BMS's statement of a "third leg" of R&D sitting alongside biology and chemistry (www.mckinsey.com.br) hints at ambitions: AI will not be an afterthought but as fundamental as lab equipment.

Expected Outcomes

If predictions hold, BMS expects more AI-designed candidates to advance to proof-of-concept. Its leaders envision that within a few years, AI will significantly improve late-stage predictions (safety, developability) ([43] www.bms.com). The ultimate goal is to turn what once took decades into what might be done in a few years. Early trials like the phase I HbF inducer suggest this is plausible. However, BMS remains measured: *"We've already been very successful at early phases; replicating that in later phases will take time and more data,"* as one executive noted.

Conclusion

BMS's "Predict First" initiative exemplifies how a large pharmaceutical company is systematically reorienting R&D around AI-human collaboration. Through clear internal messaging, bold partnerships, and tangible pilot projects, BMS portrays AI as a powerful **decision-support ally** rather than mere factory automation. The company's leaders repeatedly stress that

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integrating AI is about *enhancing scientific decision-making* – from target selection through trial design – by leveraging predictive models alongside expert judgment ([3] www.bms.com) ([9] www.pharmavoice.com).

Evidence from BMS's pipeline shows that this approach yields real benefits: molecules with AI guidance are entering clinical trials, timelines are shrinking, and productivity per scientist is rising ([18] www.bms.com) (www.mckinsey.com.br). International industry watchers note that as of 2024, no wholly AI-originated drug has yet been approved, underscoring that human oversight remains essential. BMS's stance – promoting an AI-augmented but scientist-centric R&D process – aligns with this reality and positions the company for sustained innovation.

Looking ahead, BMS envisions AI capabilities continuing to grow. As Sheth dreams of *"design [ing] biotherapeutic molecules in silico… to get to the therapeutic much faster,"* the company invests in better models, richer data, and dynamic human–AI workflows ([60] www.bms.com). If successful, BMS will have shortened drug timelines, improved success probabilities, and delivered more medicines to patients sooner. The "Predict First" paradigm thus represents not just a technological shift, but a cultural one: one that redefines drug discovery as a **predictive science** powered by "human intelligence with AI" rather than a blind search through possibility space ([2] www.bms.com) ([9] www.pharmavoice.com).

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