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*Review Article*

# Applications of Data Analysis and Artificial Intelligence Agents in Novel Drug Discovery: A Critical Literature Review

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**Abstract:** The traditional drug discovery and development process is historically characterized by high attrition rates, escalating financial costs, and decade-long timelines. The emergence of artificial intelligence (AI) and machine learning (ML) has transformed this paradigm by enabling efficient navigation through vast chemical spaces and the integration of complex multi-omic datasets. This evidence-based literature review critically examines the evolution and application of computational technologies across the pharmaceutical pipeline, ranging from early expert systems like DENDRAL, computer-aided drug design (CADD), and quantitative structure-activity relationship (QSAR) modeling to AlphaFold 3 biomolecular complex predictions, computer-assisted synthesis planning (CASP), natural product bioprospecting, and autonomous multi-agent systems. Key advancements in antimicrobial screening, precision oncology, phytochemical characterization, and clinical-stage AI-generated molecules are highlighted. Finally, the translational gap is addressed, emphasizing that AI functions as an advanced decision-support framework requiring rigorous in vitro and in vivo experimental validation, wherein qualified human mediation remains indispensable for therapeutic success.

**Keywords:** Drug Discovery; Artificial Intelligence; Machine Learning; Natural Products; Autonomous Agents.

## 1. Introduction

Bringing a new drug from the bench to the pharmacy shelf has long been one of the most punishing endeavors in modern science. The traditional pharmaceutical research and development (R&D) pipeline is notoriously slow, frequently dragging beyond ten years while consuming around 2.6 billion dollars per approved molecule [1, 2, 11]. Worse still, nine out of ten candidate molecules that show promise in early testing ultimately founder when face-to-face with human clinical trials, usually doomed by poor efficacy or unforeseen toxic effects [1, 2, 11]. As global health threats such as drug-resistant superbugs and complex cancers become more serious, a model with such a high failure rate is no longer sustainable. [1, 2, 12].

In this context, artificial intelligence (AI) has emerged not just as a new technology, but as a practical necessity [1, 2, 12]. Modern algorithms can explore chemical spaces containing an unimaginable $10^{60}$ possible structures while integrating different types of biological data, from genomic signatures to proteomic maps [1, 3, 4, 12, 13]. By moving beyond static, old-school computational models toward dynamic Machine Learning (ML) and Deep Learning (DL) architectures, researchers can now catch non-linear biological nuances that previously slipped through the cracks. This shift has markedly sharpened the ability to forecast absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties long before a single wet-lab experiment is run [2, 4, 12].

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More recently, the rise of Generative AI (GAI) and self-directed multi-agent networks operating directly alongside bench scientists (lab-in-the-loop) has reshaped what automated discovery looks like [1, 5, 14]. These agent-driven platforms do not merely respond to prompts; they read through hundreds of papers, propose biological mechanisms, and process raw flow cytometry or transcriptomic files in minutes, taking a massive cognitive load off human researchers and speeding up drug repurposing efforts [5].

Yet, despite a growing roster of AI-refined and de novo designed molecules advancing into Phase 1, 2, and 3 clinical trials [1, 3, 28, 29], a closer look at the field reveals a persistent "translational gap" [2, 15]. The vast majority of algorithmic victories remain confined to retrospective computer simulations [2, 15]. Data bias, missing metadata standards, risk of model overfitting, and the frustrating "black-box" nature of deep neural networks still stand as formidable hurdles [2, 4, 15].

This review takes a critical, evidence-grounded look at how data analysis and autonomous AI agents are reshaping drug discovery. The analysis traces the trajectory from early rule-based systems to state-of-the-art multi-agent generative networks, sifting through practical wins, real-world constraints, and the road ahead for pharmaceutical innovation [1-6].

## 2. Methods

This study was designed as a narrative review based on existing evidence to systematically map and scrutinize the deployment of AI, ML, and autonomous agent frameworks in drug discovery workflows [2, 5, 10].

The literature search targeted three main electronic portals: PubMed/MEDLINE, SciELO, and LILACS (accessed through the Virtual Health Library - VHL) [2, 5, 7]. While focusing primarily on studies published between 2018 and 2026, foundational older papers were selectively included to preserve proper historical context [2, 4, 25-30].

Search queries relied on Medical Subject Headings (MeSH) and Descritores em Ciências da Saúde (DeCS) combined with Boolean operators (AND, OR). Key search terms included: Drug Discovery, Artificial Intelligence, Machine Learning, Deep Learning, Autonomous Agents, Natural Products, Drug Repurposing, and Virtual Screening [2, 5].

To be included, publications met three specific criteria: (1) Original research or literature reviews exploring algorithmic deployment in pharmaceutical R&D; (2) Studies offering experimental (in vitro, in vivo, or clinical) validation of AI-derived candidates or natural bioactive extracts; and (3) Availability of the complete text in English or Portuguese [1, 3, 5, 7].

Incomplete drafts, non-peer-reviewed notes, and papers applying AI to non-pharmaceutical topics were excluded [2]. The gathered data were categorized into three analytical themes: (a) Technological foundations and historical evolution; (b) Field applications (antimicrobials, oncology, natural products, and repurposing); and (c) Methodological, ethical, and translational barriers [1-9, 12-15].

## 3. Discussion

### 3.1 Historical Evolution and Technological Foundations

The theoretical foundations of artificial intelligence date back to the mathematical models of artificial neurons formulated by McCulloch and Pitts in 1943, Alan Turing's seminal concepts on machine intelligence in 1950 [25], and the formal establishment of the field

during the 1956 Dartmouth Conference. In chemical and molecular biology, the earliest computational milestone occurred in 1965 with Stanford University's DENDRAL project [30], an expert rule-based system designed to infer molecular structures from mass spectrometry data.

By the late 1980s, neural computing emerged in molecular biology when Qian and Sejnowski [26] pioneered artificial neural networks to predict the secondary structure of globular proteins directly from primary sequence data [2, 26]. In the late 1990s, computational intelligence entered pharmacological response forecasting, as demonstrated by El-Deredy et al. [27], who trained artificial neural networks on nuclear magnetic resonance (NMR) spectroscopy data to predict chemotherapeutic responses in human glioma cell cultures [9, 27].

Modern bioinformatic architectures now rely on a structured hierarchy progressing from classical Machine Learning to Deep Learning and autonomous multi-agent networks [2, 4, 12, 13]. Supervised ML methods remain widely employed: Support Vector Machines (SVM) project chemical parameters into multidimensional spaces to define separating hyperplanes between active and inactive molecules, while Random Forest (RF) ensembles aggregate decision trees to handle noisy data and rank critical molecular descriptors [2, 4, 6].

Deep Learning extends these capabilities by utilizing multi-layered neural networks to extract non-linear representations from biological datasets [2, 4, 6]. Convolutional Neural Networks (CNNs) analyze 3D protein structures and density maps, whereas Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) architectures process sequential data, such as amino acid chains or Simplified Molecular-Input Line-Entry System (SMILES) strings [2, 4, 6, 14]. More recently, Graph Neural Networks (GNNs) have gained prominence by modeling molecules directly as mathematical graphs (atoms as nodes, bonds as edges), preserving stereochemical and topological information [1, 2, 6].

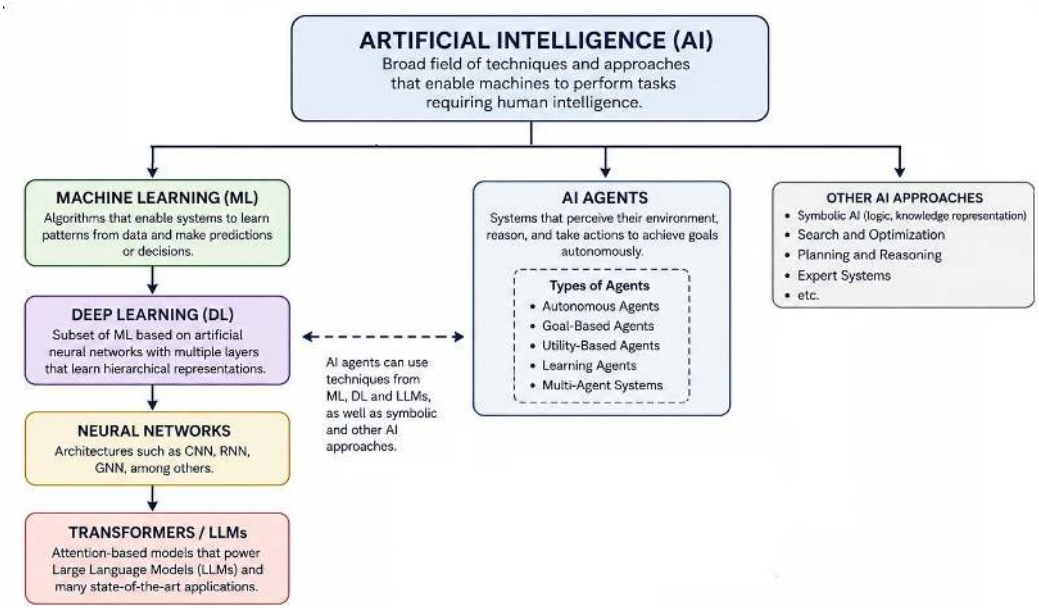



**Figure 1.** Main concepts and subfields of Artificial Intelligence

### 3.2 CADD, QSAR Modeling, and Virtual Screening

Computer-Aided Drug Design (CADD) is divided into Structure-Based Drug Design (SBDD) and Ligand-Based Drug Design (LBDD) methodologies [2, 4]. When target 3D structures are available, via crystallography, Nuclear Magnetic Resonance (NMR), or deep learning predictions such as AlphaFold 2 [16], Structure-Based Virtual Screening (SBVS) employs molecular docking to evaluate ligand-receptor binding energies [2, 4]. The groundbreaking release of AlphaFold 2 and its complete mapping of the human proteome revolutionized structural biology, earning its principal architects the 2024 Nobel Prize in Chemistry. Crucially, the advent of AlphaFold 3 in 2024 [31] expanded predictive fidelity beyond isolated proteins to model multi-component complexes, accurately predicting joint structural interactions between proteins, nucleic acids (DNA/RNA), post-translational modifications, and small-molecule ligands [31].

When target tertiary structures are absent, LBDD utilizes Ligand-Based Virtual Screening (LBVS) and Quantitative Structure-Activity Relationship (QSAR) modeling to mathematically link physicochemical descriptors with experimental bioactivity (pIC50) [2, 4].

To address synthetic tractability in de novo molecular generation, Computer-Assisted Synthesis Planning (CASP) integrates Monte Carlo Tree Search (MCTS) with deep neural networks trained on historical reaction databases [6]. CASP evaluates retrosynthetic pathways, iteratively decomposing target molecules into commercially accessible precursors within seconds [6].

### 3.3 Autonomous AI Agent Architectures and Orchestration

A recent advancement in biomedical AI is the transition from isolated predictive models to Autonomous AI Agents [5, 7]. Unlike traditional generative architectures that rely on continuous user prompting, autonomous agents exhibit self-directed planning, task execution, and workflow orchestration [5, 7]. Santos and Aganette [7] demonstrate that computational agents can autonomously read literature, extract analytical categories, and structure complex findings, adapting their behavior over time [7].

In drug discovery, agents combine Large Language Models (LLMs) with code execution environments (Python/R) and specialized scientific tools [5, 7]. A prominent example is the Robin multi-agent architecture [5]. Operating within a lab-in-the-loop framework, Robin integrates specialized sub-agents: (a) Literature Agents (Crow and Falcon) that perform automated retrieval across PubMed, Open Targets, and patent libraries to formulate and rank therapeutic hypotheses; and (b) Data Analysis Agent (Finch) that autonomously generates and executes Python scripts in Jupyter Notebooks to analyze raw transcriptomic and flow cytometry data, using processed insights to refine subsequent experimental cycles [5].

This multi-agent workflow enabled Robin to synthesize 551 scientific articles in 30 minutes, reducing human cognitive labor from roughly 400 hours to under 2 hours per discovery iteration [5].

### 3.4 Applications Along the Pharmaceutical Pipeline

#### 3.4.1 Antibiotic Discovery and Resistance Management

Antimicrobial resistance creates an urgent need for new drugs [2, 8]. Stokes et al. [2, 6] trained a Directed Message Passing Neural Network (D-MPNN) on Escherichia coli growth inhibition data. Screening over 100 million compounds from the ZINC15 database [17] identified Halicin, a molecule with a unique structure that showed strong

activity against multidrug-resistant Acinetobacter baumannii and Clostridioides difficile in vivo [2, 6].

In research on Mycobacterium tuberculosis, Kouchaki et al. [8] analyzed 13,402 clinical isolates from around the world. Their machine learning model, which combined Gradient Tree Boosting (GBT) with Sparse PCA, performed better than existing molecular diagnostic methods. It improved the prediction AUC by 23.1% for pyrazinamide and 15.2% for ciprofloxacin and also identified new genomic variants linked to drug resistance [8].

#### 3.4.2 Precision Oncology, Single-Cell Omics, and Drug Synergy

Cancer treatments using a single drug often fail because of differences between cancer cell groups and the development of drug resistance [1, 9]. Computational tools such as DeepSynergy combine gene expression data from cancer cell lines with chemical information to predict effective drug combinations. These combinations can reduce the required drug doses and decrease toxicity to healthy tissues [9, 18].

Furthermore, single-cell RNA sequencing (scRNA-seq) combined with deep learning models such as Dr.VAE [19] helps researchers study changes in different cell groups and assess how drugs affect resistant cells. This approach supports the development of drug combinations that target diverse cancer cell populations [9, 19].

#### 3.4.3 Drug Repurposing and Clinical Translation

Drug repurposing uses approved drugs with known safety and pharmacokinetic profiles in humans, as documented in resources such as DrugBank [20] [1, 2, 5]. The Robin system identified increased retinal pigment epithelium (RPE) phagocytosis as a potential treatment strategy for dry age-related macular degeneration (dAMD) and identified ripasudil, an approved glaucoma drug, as a possible treatment [5]. In vitro tests showed a 1.89-fold increase in phagocytosis and increased ABCA1 expression, suggesting a new mechanism of action [5].

The clinical testing of AI-designed molecules has reached important milestones. In 2020, DSP-1181 (developed by Exscientia and Sumitomo), entered clinical trials for obsessive-compulsive disorder as the first AI-designed small molecule tested in humans. Its preclinical development was completed in only 12 months [28]. Later, Rentosertib (ISM001-055), developed by Insilico Medicine, entered Phase 2 trials for idiopathic pulmonary fibrosis in 2023. It was the first drug for which both the biological target and chemical structure were discovered entirely using generative AI [29]. Several other AI-optimized molecules have also advanced to clinical trials, as summarized in Table 1 [1, 3].

**Table 1.** Representation of AI-designed or AI-optimized drug candidates in clinical trials.

| Candidate / Code | Developer / Company | Indication | Target / Mechanism of Action | Clinical Status / Phase |
|---|---|---|---|---|
| Rentosertib (ISM001-055) | Insilico Medicine | Idiopathic Pulmonary Fibrosis | De novo designed small molecule against novel AI target | Phase 2 [29] |
| DSP-1181 | Exscientia / Sumitomo | Obsessive-Compulsive Disorder | Serotonin 5-HT1A agonist (preclinical done in 12 months) | Phase 1 (Pioneer) [28] |
| REC-2282 | Recursion Pharmaceuticals | Neurofibromatosis Type 2 | Oral/CNS-permeable HDAC inhibitor | Phase 2/3 [3] |
| RLY-4008 | Relay Therapeutics | Solid Tumors | Highly selective FGFR2 inhibitor | Phase 2 [3] |
| BPM31510 | BERG Health | Solid Tumors / Oncology | Cellular metabolic machinery modulator | Phase 2 [3] |
| EXS-21546 | Exscientia / Evotec | Solid Tumors (NSCLC, Renal) | Selective Adenosine A2A receptor antagonist | Phase 1 [1, 3] |
| PHI-101 | Pharos iBio | Ovarian & Breast Cancer | Chk2 / FLT3 Tyrosine Kinase inhibitor | Phase 1 [3] |

*Source: Synthesized and adapted from Shahzad et al. [3], Hopkins et al. [28], and Ren et al. [29].*

#### 3.4.4 Virtual Screening of Natural Products, Phytocompounds, and Essential Oils

Natural products and their secondary metabolites have long been important sources of bioactive compounds [1, 4]. However, traditional screening of complex plant materials, such as crude extracts, fractions, and essential oils containing monoterpenes and sesquiterpenes, can be challenging due to the high costs of compound isolation and the difficulty of understanding their mechanisms of action [1, 4].

Machine learning connects natural compound databases, such as PubChem [21] and ChEMBL [22], with disease targets using molecular docking, SwissADME analysis [23], and ProTox-II toxicity screening [24] [4]. In addition, AI models can analyze interactions between multiple compounds in plant mixtures and predict how different essential oil components work together across biological pathways. This can help optimize antimicrobial or cytotoxic effects while assessing their ADMET safety profiles [1, 4, 9, 10, 23, 24].

### 3.5 Persistent Challenges and the "Translational Gap"

Despite computational efficiency gains, AI implementation encounters substantive methodological barriers [2, 4, 15]. Bin Abdulqader et al. [2] emphasize a persistent "translational gap", wherein the majority of AI-driven findings remain confined to in silico evaluations [2].

Machine learning performance depends on the quality and representativeness of the data [2, 4, 15]. Public bioactivity databases often contain experimental errors, differences in testing methods, and publication bias against inactive compounds [2, 4, 15]. In addition, deep neural networks can act as "black boxes", making it difficult to understand the reasons behind their predictions. This lack of transparency can also make regulatory evaluation more challenging for agencies such as the FDA and ANVISA [2, 4, 15].

Ultimately, AI does not replace empirical pharmacology [2]. As Bin Abdulqader et al. [2, p. 17] emphasize:

> *"While AI models can be fast in generating structurally novel and theoretically active compounds, confirming their biological efficacy, synthetic accessibility, and clinical safety remains entirely dependent on conventional experimental workflows."*

AI functions primarily as a decision-support system; definitive validation requires wet-lab assays, in vivo testing, and controlled clinical trials [2, 5, 7].

## 4. Conclusion

Integrating big data analytics, deep neural networks, and autonomous AI agents into pharmaceutical R&D represents a significant advance in biomedical discovery, accelerating early-stage screening, retrosynthetic design, and drug repurposing [1, 4, 5, 12, 13].

However, bridging the translational gap requires standardized data governance, explainable AI architectures, and continuous integration with laboratory workflows [2, 15]. Artificial intelligence will not replace biomedical researchers; rather, scientists who effectively and critically utilize these computational frameworks will drive future therapeutic innovations [2, 7, 15].

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