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Artificial Intelligence in Drug Repurposing: Current Advances, Challenges, and Future Perspectives for Precision Medicine

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ABSTRACT

Background: Traditional drug discovery is constrained by exorbitant costs, extended development timelines, and high clinical attrition rates. Applying artificial intelligence (AI) to drug repurposing offers an efficient strategy to accelerate therapeutic discovery, lower financial barriers, and advance precision medicine. However, stakeholder perspectives regarding its practical integration and challenges remain insufficiently characterised.

Methods: We administered a cross-sectional, questionnaire-based survey to evaluate public and professional awareness, perceived limitations, and ethical considerations surrounding AI-driven drug repurposing. Using a convenience sampling approach, quantitative data were gathered from N=118 respondents representing diverse demographic cross-sections (63.6% female, 34.7% male; 52.5% aged 18–24) and education levels (44.9% undergraduate, 35.6% postgraduate). Descriptive and percentage-based statistical analyses were executed to evaluate familiarity, primary bottlenecks, and governance preferences.

Results: While general AI awareness reached 100%, familiarity with computational drug repurposing was 50.8% n=60). Respondents identified data privacy concerns (26.3%) and algorithm bias (22.9%) as primary computational hurdles. Furthermore, a shortage of skilled interdisciplinary professionals (30.5%) and a deficit in public trust (29.7%) were highlighted as the main adoption bottlenecks. Regarding clinical execution, 44.9% favoured physician decision-making supported by AI systems, while 55.1% projected that AI-guided repurposing will achieve widespread adoption within the next decade.

Conclusion: Although confidence in AI's transformative impact on precision medicine is high, widespread implementation requires mitigating data privacy risks, building algorithmic transparency, and training cross-disciplinary specialists. Human-in-the-loop clinical frameworks remain essential to ensure safe, ethically aligned adoption.

Keywords: Computational Pharmacology, Drug Repositioning, Machine Learning in Healthcare, Pharmacomics, Algorithmic Bias, Human-in-the-Loop Clinical Decision-Making, Technology Acceptance Survey.

INTRODUCTION

Modern healthcare is being squeezed from two directions at once: diseases are growing more complex to treat, while the process for developing new therapies to treat them has barely sped up to match. A single new chemical entity still typically takes ten to seventeen years and $2 billion to $3 billion to reach approval, and most candidates never make it, often failing late in clinical testing once problems with toxicity or efficacy finally surface. Repurposing an already-approved or previously investigated drug sidesteps much of that risk, since its safety and pharmacokinetic profile is already on record; this alone can compress development to three to twelve years at a fraction of the cost, often closer to $300 million [5]. What has changed the calculus more recently is artificial intelligence. Algorithms capable of mining chemical, genomic, and clinical data at a scale no human team could match are now being layered onto repurposing pipelines, and this convergence is unfolding just as precision medicine — treatment tailored to a patient's genetic and physiological profile — moves from aspiration to expectation across much of modern therapeutics. [4], [16], [20]

The literature reviewed for this study traces how that convergence has taken shape. Foundational work by Pushpakom et al. [6] mapped out the rationale, validation pathways, and practical obstacles of systematic repurposing well before AI became central to the conversation, and much of what followed has built on that groundwork rather than replaced it. Once machine learning entered the picture, attention shifted toward

what the algorithms could actually do: supervised models, graph-based architectures, and more recently generative and language-based tools have been used to accelerate virtual screening, predict drug–target interactions, and mine biomedical text and clinical databases for repurposing candidates [1], [21], [30]. A closely related thread ties this methodological progress to precision medicine specifically, using pharmacogenomic and multi-omics data, or electronic health records paired with machine-learning platforms, to match repurposed compounds to the patients most likely to benefit [2], [10], [36], [43]. The same pairing shows up repeatedly in disease-specific work: AI-guided repurposing has been explored for oncology and multiple sclerosis [11], [26], for glioblastoma [22], and, notably, for orphan and rare diseases, where the sheer scarcity of treatment options makes even modest repurposing gains disproportionately valuable [19], [35]. Running underneath all of this is a broader, healthcare-wide literature that situates drug repurposing within AI's larger footprint in medicine — diagnostics, treatment planning, system efficiency — while consistently flagging the same handful of concerns: data privacy, algorithmic opacity, and a healthcare infrastructure not yet built to absorb these tools at scale [8], [9], [12]. [23], [33], [42]

What this body of work says comparatively little about, though, is who is actually expected to trust, adopt, and work alongside these systems. A few of the reviews above acknowledge, usually in a closing paragraph on challenges, that data quality, algorithmic transparency, and a shortage of interdisciplinary talent will decide whether AI-guided repurposing survives contact with real clinical practice [23], [33], [42], yet none of the sources examined here actually measure those concerns among the people they concern: patients, clinicians, students, or the wider public whose confidence the technology ultimately depends on. There is no quantified account of how aware non-specialists are of computational repurposing relative to their awareness of AI in general, how much they trust an AI-supported clinical decision against one made by a physician alone, or which governance model they would find acceptable. That gap is not a minor omission. A technology whose real-world uptake hinges on regulatory approval and public trust cannot be judged on algorithmic performance alone, and without baseline data on where stakeholders currently stand, calls to "build trust" or "train interdisciplinary talent" remain well-intentioned guesses rather than evidence-based priorities. This study is designed to close that gap: rather than adding another technical benchmark to an already crowded field, it reports primary, cross-sectional survey data on where public and professional confidence in AI-driven drug repurposing currently sits. [3], [7], [18], [31], [32], [41]

Accordingly, this study set out to characterise awareness, perceived technical and ethical barriers, and governance preferences surrounding AI-driven drug repurposing among a demographically varied group of respondents, and to see how those attitudes align — or fail to align — with the confidence expressed in the technical literature summarised above. Its specific objectives were threefold: to measure baseline familiarity with computational repurposing against general AI awareness; to identify which technical, ethical, and operational barriers respondents rank as most pressing; and to capture stakeholder preferences for clinical decision-making models, regulatory oversight, and the pace at which they expect these tools to reach routine use. Read alongside the algorithmic advances already documented in the field, this evidence is meant to give researchers, educators, and policymakers a more human-centred basis for the safeguards, training programmes, and oversight structures that AI-guided repurposing will need going forward. The gap that matters most, in the end, is not computational but human: the distance between what these systems can already do and what patients, clinicians, and regulators are ready to accept. Closing it will determine whether AI-driven repurposing shortens the path from a promising algorithm to a therapy someone can actually receive. [14], [34], [37], [39], [40]

LITERATURE REVIEW:

1. Economic and Operational Drivers in Drug Discovery: *De Novo* vs. Drug Repurposing

Traditional *de novo* therapeutic discovery operates under severe economic and temporal constraints. Standard drug development pipelines require an average capital investment ranging from $2 billion to $3 billion and span 10 to 17 years per newly approved chemical entity. High attrition rates further hamper this process during early clinical phases, in which approximately 89% of drug candidates fail due to unexpected toxicity, unfavourable pharmacokinetics, or insufficient clinical efficacy. Fields such as neurodegeneration, oncology, and orphan diseases experience particularly high failure rates during late-stage trials. [5], [16], [20], [25]

To circumvent these structural barriers, drug repurposing—or drug repositioning—has gained prominent traction as a viable alternative. By identifying novel therapeutic indications for previously approved, investigational, or discontinued compounds, repurposing capitalises on pre-existing safety, pharmacokinetic, and toxicological data. Consequently, development timelines are compressed to 3 to 12 years, and capital expenditure is reduced to roughly $300 million per asset. This de-risked strategy provides an expedited pathway to address unmet medical needs, manage emerging infectious outbreaks, and develop therapies for rare diseases [6], [7], [35]

2. Methodological Evolution: From Classical Repurposing to AI-Driven Pipelines

Historically, drug repositioning relied on serendipitous clinical observations, target homology analysis, or

low-throughput phenotypic screening. While successful in landmark cases, these trial-and-error approaches were inherently limited in scale and biological scope. The influx of high-throughput bio-data—encompassing genomics, transcriptomics, metabolomics, and electronic health records (EHRs)—has catalysed a transition toward systematic computational repurposing pipelines. [3], [20], [21], [30], [32]

Artificial intelligence (AI) and machine learning (ML) algorithms have reorganised these informatics workflows. Supervised machine learning models, graph neural networks (GNNs), and deep learning architectures excel at processing high-dimensional biological networks, predicting drug-target interactions (DTIs), and evaluating binding affinities across vast chemical libraries. Combining AI with high-throughput virtual screening has been demonstrated to reduce early-stage screening timelines by 30% to 50% while improving candidate hit rates compared to traditional wet-lab assays. Furthermore, recent developments in generative AI and Natural Language Processing (NLP) enable automatic text mining of biomedical literature, mining of clinical databases, and structure-activity relationship (SAR) profiling. [1], [16], [25], [31], [32], [39], [45]

3. Intersecting AI Repurposing with Precision Medicine

Precision medicine aims to tailor therapeutic interventions to individual patient characteristics by factoring in genetic variations, environmental exposures, and real-time physiological markers. Traditional disease management often relies on uniform treatment protocols, which can result in sub-optimal therapeutic responses or adverse drug reactions (ADRs) across heterogeneous populations. Integrating AI-driven drug repurposing with precision medicine strategies allows therapeutic candidates to be evaluated against specific sub-populations rather than broad, unstratified cohorts. [2], [10], [13], [15], [17]

Recent advances in pharmacogenomics (PGx) and next-generation sequencing (NGS) provide deep molecular datasets that inform targeted drug repositioning. Machine learning algorithms process multi-layer omics data to discover predictive biomarkers, delineate disease subtypes, and identify subpopulation-specific drug targets. For instance, in complex pathologies such as glioblastoma, neurodegenerative disorders, and orphan diseases, AI frameworks analyse individualised molecular profiles to pair existing drug scaffolds with newly identified biological targets. By aligning computational drug repositioning with individual genetic and phenotypic profiles, researchers can optimise therapeutic efficacy, reduce toxicity risks, and improve clinical trial design. [15], [17], [24], [27], [28], [29], [36], [37], [38], [43], [44]

4. Computational, Ethical, and Translational Bottlenecks

Despite the theoretical and technical capabilities of AI-driven drug repurposing, several translational hurdles complicate its integration into routine pharmaceutical and clinical workflows. From a computational standpoint, AI models are susceptible to data quality limitations, including missing clinical values, batch effects in high-throughput omics data, and selection bias within public databases. Furthermore, many deep learning models operate as opaque "black boxes," lacking algorithmic interpretability. This lack of transparency can make it difficult for clinical researchers to decipher the underlying mechanistic rationale behind predicted drug-target interactions. [8], [9], [12], [18], [23], [33], [41], [42]

From a legal and regulatory perspective, data privacy risks remain a paramount concern when utilising sensitive patient records, genomic profiles, and electronic health information. Issues surrounding intellectual property (IP) rights, patent eligibility for newly discovered indications of off-patent drugs, and liability for AI-informed clinical errors present unresolved regulatory questions. Furthermore, operational bottlenecks include a persistent shortage of interdisciplinary specialists fluent in both computational data science and molecular pharmacology, alongside variable public and institutional trust in AI-driven healthcare interventions. Addressing these challenges requires human-in-the-loop decision-making frameworks, clear regulatory guidelines, and robust stakeholder engagement to bridge the gap between algorithmic predictions and safe clinical deployment. [14], [18], [31], [34], [40], [44]

METHODOLOGY:

Materials and Methods

Research Design

This study utilised a quantitative, cross-sectional survey design to evaluate baseline awareness, perceived computational limitations, ethical priorities, and governance preferences regarding artificial intelligence (AI) in drug repurposing and precision medicine. Primary empirical data were collected from $N = 118$ respondents across diverse demographic sectors. A convenience sampling strategy was used to capture perspectives across different educational levels, age groups, and occupational backgrounds, providing a broad assessment of public and professional attitudes toward computational therapeutics.

Materials and Datasets

Data collection was executed using a structured online survey developed and hosted on the Google Forms platform. The instrument comprised 25 standardised items categorised into four key sections:

- **Demographics:** Participant age, gender, educational qualification, and primary occupation.
- **Awareness and Technical Familiarity:** General AI familiarity, computational drug repurposing awareness, primary information sources, and specific technological domain exposure (e.g., machine

learning, generative AI, graph neural networks).

- **Perceived Limitations and Ethical Concerns:** Algorithmic bias, data privacy, cybersecurity risks, transparent decision-making, and adoption bottlenecks.
- **Clinical Execution and Future Implementation:** Preference for human-in-the-loop decision-making, regulatory oversight, and projected adoption timelines within precision medicine.

Methods and Procedures

The survey was distributed digitally via academic channels, professional networks, and social media platforms to reach a broad demographic cross-section.

1. **Administration:** Participants accessed the questionnaire asynchronously through a secure web link generated by Google Forms.
2. **Completion:** Responses were collected over the survey period. Submission required completing all mandatory multiple-choice and multi-select items to prevent missing values.
3. **Extraction:** Raw numerical and categorical response matrices were extracted directly from Google Forms in tabulated Excel format (.xlsx) for downstream processing.

Analytical Tools and Software

Data processing, statistical evaluation, and data visualisations were performed using the following software platforms:

- **OriginPro:** Conducted descriptive statistical calculations, frequency distributions, percentage calculations, and produced publication-ready charts and comparative figures.
- **Generative AI Platforms (ChatGPT and Google Gemini):** Utilised as computational writing and analytical support tools to organise text formatting, refine qualitative explanations, and assist in structuring analytical summaries based on the raw empirical data.

Ethical Considerations and Governance

Participant privacy and research ethics were maintained throughout the study:

- **Voluntary Participation & Consent:** Participation was completely voluntary. Clear information regarding the study's objective was provided at the beginning of the survey, and proceeding to complete the questionnaire served as informed consent.
- **Anonymity & Confidentiality:** No personally identifiable information (PII)—such as names, email addresses, or IP addresses—was requested or stored. All responses were collected and analysed anonymously.
- **Data Protection & Mitigation of Bias:** Raw data files were stored securely on password-protected local systems accessible only to the research team. Potential selection bias inherent to convenience sampling was addressed by reporting demographic breakdowns transparently across all analysed sub-groups.

RESULTS AND DISCUSSION:

Results:

Demographic and Baseline Awareness Distribution

The survey dataset comprised $N = 118$complete individual submissions. Within the sample, 63.56% ($n = 75$) identified as female, 34.75% ($n = 41$) as male, and 1.69% ($n = 2$) preferred not to disclose gender identity. Age breakdown revealed that the majority of participants were aged 18–24 years (52.54%, $n = 62$), followed by those aged 45–54 years (24.58%, $n = 29$). Regarding educational attainment, undergraduates accounted for 44.92% ($n = 53$) of respondents, while postgraduates represented 35.59% ($n = 42$).

While general awareness of artificial intelligence achieved a 100.00% baseline ($n = 118$), specific familiarity with computational drug repurposing was recorded at 50.85% ($n = 60$).

Perceived Technical Hurdles and Operational Bottlenecks

Participants evaluated technical barriers to AI integration in drug discovery. Data privacy concerns emerged as the primary computational challenge, cited by 26.27% ($n = 31$) of respondents. Algorithmic bias and poor data quality were equally prioritized, each selected by 22.88% ($n = 27$) of the cohort. Regulatory constraints (16.10%, $n = 19$) and a lack of algorithmic transparency (11.86%, $n = 14$) constituted the remainder of technical challenges.

Regarding broader operational adoption barriers, respondents identified a shortage of skilled interdisciplinary professionals as the primary limitation (30.51%, $n = 36$). A deficit in public or clinical trust ranked second at 29.66% ($n = 35$), followed by poor data availability (16.95%, $n = 20$) and high implementation costs (16.10%, $n = 19$).

Clinical Governance, Risk Priorities, and Projections

When evaluating decision-making frameworks, 44.92% ($n = 53$) favored a "physician assisted by AI" approach. Independent decision-making by physicians without AI involvement was preferred by 33.05% ($n = 39$), whereas fully autonomous AI decision-making received 2.54% support. Regarding regulatory structures, 39.83% ($n = 47$) advocated for shared oversight involving government agencies, pharmaceutical

entities, and clinical institutions.

The primary concern regarding clinical AI implementation was the risk of wrong predictions (58.47%), with rigorous clinical validation cited as the most critical prerequisite (35.59%) prior to clinical acceptance. Rare diseases (33.90%) and oncology (25.42%) were identified as the therapeutic areas positioned to benefit most from computational drug repositioning. Looking ahead, 55.08% ($n = 65$) projected that AI-guided drug repurposing will achieve widespread clinical integration within the next decade, while 39.83% ($n = 47$) expressed uncertainty.

Table 1: Key Survey Metrics and Percentage Distributions ($N = 118$)

Survey Domain	Category / Response Option	Count (n)	Percentage (%)
Demographics	Female	75	63.56%
	Male	41	34.75%
	Prefer Not to Say	2	1.69%
	Age: 18–24 Years	62	52.54%
	Age: 45–54 Years	29	24.58%
	Undergraduate Level	53	44.92%
	Postgraduate Level	42	35.59%
Awareness Baseline	General AI Awareness (Yes)	118	100.00%
	Drug Repurposing Awareness (Yes)	60	50.85%
Primary Technical Hurdles	Data Privacy Concerns	31	26.27%
	Algorithmic Bias	27	22.88%
	Poor Data Quality	27	22.88%
	Government Regulations	19	16.10%
	Lack of Algorithmic Transparency	14	11.86%
Adoption Bottlenecks	Shortage of Skilled Professionals	36	30.51%
	Lack of Public / Clinical Trust	35	29.66%
	Poor Data Availability	20	16.95%
	High Implementation Cost	19	16.10%
Governance & Decision-Making	Doctor with AI Support (Human-in-the-Loop)	53	44.92%
	Physician Operating Independently	39	33.05%
	Shared Regulation (Government + Industry + Academia)	47	39.83%
10-Year Clinical Projection	Widespread Adoption Likely (Yes)	65	55.08%
	Uncertain / Undecided	47	39.83%

DISCUSSION:

Interpretation and Comparison with Literature

The stark divergence between universal general AI awareness (100.00%) and specific drug repurposing familiarity (50.85%) underscores a broader educational gap between general technological literacy and specialised bioinformatics concepts. While published computational literature emphasises the theoretical acceleration of virtual screening—where algorithms reduce screening timelines by 30% to 50%—the empirical data demonstrate that real-world integration depends heavily on addressing ethical, operational, and structural constraints. [2], [3], [10], [13], [15], [17], [24], [28], [29], [36], [37], [38], [43], [44]

The prioritisation of data privacy (26.27%), algorithmic bias (22.88%), and data quality (22.88%) aligns directly with bioethical research warning against the uncritical deployment of opaque models in precision healthcare. Furthermore, the strong stakeholder preference for physician-guided AI support (44.92%) over fully autonomous systems (2.54%) mirrors recent bioethical frameworks advocating for human-in-the-loop decision architectures. This consensus reflects a deliberate caution toward algorithmic error, supported by

the finding that 58.47% of respondents identified wrong predictions as their foremost concern. [8], [9], [12], [18], [23], [31], [41]

The operational bottleneck highlighted by respondents—specifically the acute shortage of skilled interdisciplinary professionals (30.51%)—corroborates informatics literature stressing that translating in silico predictions into clinical outcomes requires dual proficiency across data science and molecular pharmacology. [7], [14], [20], [21], [30], [33], [34], [42]

Limitations:

Several methodological parameters qualify these findings:

1. **Sampling Bias:** Convenience sampling via digital forms resulted in a sample skewed toward younger demographics (52.54% aged 18–24) and academic cohorts, which may not fully reflect clinical practitioner or regulatory perspectives.
2. **Geographic Uniformity:** The survey dataset lacks geographical and health-system stratification, limiting direct extrapolation across differing regulatory jurisdictions or low-resource settings.
3. **Self-Reported Metrics:** Measures of technical awareness and perceived risks rely on self-reported evaluations rather than standardised objective knowledge metrics.

Implications and Significance

These empirical findings carry clear actionable implications for policy, education, and clinical practice:

- **Governance Strategy:** The demand for shared oversight (39.83%) indicates that regulatory frameworks must involve multi-stakeholder collaboration among government, industry, and healthcare institutions to foster public trust.
- **Curriculum Reform:** Addressing the primary adoption bottleneck requires higher education institutions to build cross-disciplinary programs bridging computational science, pharmacology, and bioethics. [4], [5], [16], [19], [22], [25], [26], [27], [32], [35], [39]
- **Clinical Integration:** Successful deployment of AI-repurposed compounds in precision medicine depends on preserving physician oversight, establishing algorithmic transparency, and validating model outputs against rigorous real-world evidence before clinical adoption. [1], [11], [24], [28], [38], [40], [44], [8], [12], [18], [23], [41], [42]

CONCLUSION:

This research evaluated public and professional awareness, perceived computational hurdles, ethical priorities, and governance preferences surrounding artificial intelligence (AI) in drug repurposing to establish human-in-the-loop strategies for its safe integration into precision medicine.

The empirical evaluation reveals a pronounced divergence between universal general AI awareness (100.00%, $N = 118$) and specific familiarity with computational drug repositioning (50.85%). Stakeholders identified data privacy risks (26.27%), algorithmic bias (22.88%), and poor data quality (22.88%) as primary computational barriers, alongside operational bottlenecks such as a severe shortage of skilled interdisciplinary professionals (30.51%) and a deficit in public trust (29.66%). Notably, a strong human-in-the-loop consensus emerged: 44.92% of respondents advocated for physician decision-making supported by AI systems, compared to a mere 2.54% favouring autonomous AI operation. Heightened concerns over wrong predictions (58.47%) highlighted rigorous clinical validation (35.59%) as an indispensable prerequisite for adoption, with rare diseases (33.90%) and oncology (25.42%) identified as high-impact therapeutic domains. Whereas previous literature focuses heavily on theoretical model architectures and in silico benchmarks, this study provides a first-in-class empirical benchmark on multi-stakeholder readiness, ethical concerns, and clinical trust. By quantifying stakeholder demand for human-centric workflows, this work directly connects computational drug discovery to practitioner oversight, workforce development, and shared regulatory frameworks across government, industry, and academia. [3], [7], [20], [21], [30], [32], [33], [34], [39]

These contributions should be contextualised within the study's limitations, which include a digital convenience sample ($N = 118$) skewed toward younger academic demographics (52.54% aged 18–24), an absence of geographic or health-system stratification, and reliance on self-reported evaluations.

Future research should expand to multi-centre, international cohorts targeting specialised clinical subgroups, including oncologists, pharmacologists, bioethicists, and regulatory officials. Furthermore, academic institutions must establish accredited cross-disciplinary curricula bridging data science and pharmacology, alongside standardised auditing frameworks and clinical validation protocols to safely translate transparent, bias-minimised AI drug recommendations into routine bedside care. [14], [15], [17], [36], [37], [38], [40], [43], [44]

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Appendix:
Survey Questionnaire Link
https://docs.google.com/forms/d/1bneZtwtMz0__MaYA-TBlWycY6GaVIKQ-ZBnO8uoUj_o/edit