
AI IN DRUG DISCOVERY: LEGAL CHALLENGES OF LIABILITY, ACCOUNTABILITY, AND REGULATION

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ABSTRACT

The pharmaceutical industry, specifically drug discovery, has experienced a swift revaluation with Artificial Intelligence (AI) to discover more targets faster and enhance the molecular design process as well as decreasing costs and time needed to complete standard research pipelines. Although these developments hold bright potential in improving the health outcomes of the population, they are also presenting challenging legal issues with regard to liability, accountability, and regulatory controls. The drug discovery AI is based on opaque, data-intensive and frequently autonomous decision-making processes, and this makes it disruptive to the traditional legal systems that are founded on human agency, fault and evident causation. In this paper, the critical analysis of a standard of the theoretical and practical solutions applied to the issue of harms due to AI-assisted pharmaceutical development will be made to determine whether the current pharmaceutical liability structures, including product liability, negligence, and vicarious liability, can resolve arising harms. It also examines the problem of accountability gap that is proposed by black-box algorithms, dotted chains of decision-making, and the participation of various participants such as pharmaceutical firms, AI creators, data vendors, and regulators. The study assesses the developing regulatory strategies towards AI in healthcare and laments the disintegration of drug regulation and AI regulation using a doctrinal and a comparative legal analysis. The paper defends the position that the legal aspect of AI as a neutrally applied tool is insufficient in the safety-critical areas of AI drug discovery. It suggests the necessity of the system-based approach to law that includes the strict or shared liability models, increased the requirement of transparency and explainability, and the necessary AI-specific regulating measures in the pharmaceutical approval procedures. Finally, the paper argues that the legal regulation and governance of AI in drug discovery are not only the means to hold the companies accountable and compensate victims but also to achieve the confidence and moral legitimacy of the technologically-driven healthcare innovation.

Keywords: Artificial Intelligence; Drug Discovery; Pharmaceutical Liability; Accountability; AI Regulation; Product Liability; Healthcare Law

1. Introduction: AI-Driven Transformation of Drug Discovery

Traditionally, the pharmaceutical industry has used a linear-trial and error paradigm of drug discovery that is characterized by laboratory experiments, animal trials, and multi-phase clinical trials that take 10-12 years and cost billions of dollars,¹. Although this model has regulatory protection, it is still inefficient with a high failure rate and unreliable safety results. To curb these structural constraints, Artificial Intelligence (AI) has been predominantly implemented as a disruptive technology in drug discovery, so it fundamentally changes the concept, testing and commercialisation of pharmaceutical innovation.²

AI-assisted drug discovery is the alternative to intuition-driven experimentation using data-centric predictive modelling. Machine learning models are being utilised to discover biological targets based on the analysis of genomic and proteomic data and deep learning models are used to predict molecular interactions, toxicity profiles, and pharmacokinetic behaviour with an amount of speed and scale that would not be possible in humans. The current generation AI models are capable of generating new molecules and optimizing lead candidates, which significantly lowers the rate of early-stage attrition errors at AI. Drug repurposing, design of clinical trials where variable parameters, strategy through patient stratification, predictive enrolment, and outcome forecasting, are also part of AI, are also used.³

Although, such developments offer improved efficiency and cut-down in the cost of development, they also present unprecedented legal risks. Drug discovery is an area of safety critical work, such that flaws and design flaws may lead to irreparable, physical damage, epidemiological effects on the general populace, and death. In comparison with the traditional pharmaceutical decision-making, AI systems are frequently treated as black boxes, delivering results without having, in an apparent way, a rationale. This cloud is a nightmare to the regulation, judicial checks and balances, and accountability following damage, especially when the adverse drug reactions or long-term safety failures are realized after the drug has been tested and approved on the market.⁴

¹ Joseph A. DiMasi, Henry G. Grabowski & Ronald W. Hansen, "Innovation in the Pharmaceutical Industry: New Estimates of R&D Costs" (2016) 47 *Journal of Health Economics* 20.

² World Health Organization, *Ethics and Governance of Artificial Intelligence for Health* (WHO, Geneva, 2021).

³ U.S. Food and Drug Administration, *Artificial Intelligence and Machine Learning in Software as a Medical Device* (Discussion Paper, 2019).

The fact that AI-driven drug discovery is distributed also contributes to the escalation of the legal risk. The process of decision-making is not limited to one single pharmaceutical manufacturer anymore but is distributed to AI developers, data providers, contract research organisations and regulators. This fragmentation undermines fundamental law on pharmaceutical liability that conventionally attributes responsibility on identifiable human error, foreseeability, and causal relationship.⁵ In the event of damage caused as a consequence of an AI-generated prediction of molecules or based on a data-driven clinical trial outcome, the issue of legal liability will be highly disputed.

The main research issue that is sought to be tackled in this paper is as such whether there is legal responsibility in cases AI-assisted drug discovery results in injury? Should the pharmaceutical companies, as end-user, the creators of AI systems, or a combination of multiple actors all be subjected to liability in shared or strict liability regimes?⁶ The current legal systems were not planned to integrate autonomous or semi-autonomous decision systems that constantly develop on the basis of machine learning, which casts uncertainty on whether they are sufficient to meet the AI-pharmaceutical scenario.

Three major research questions understand this paper. First, do consumer harms caused by AI-based drug discovery benefit from existing pharmaceutical liability regimes, including product liability, negligence, and vicarious liability?⁷ Second, will AI systems be legally imaginised as more of a tool and under human control, or are they like more of a quasi-decision-maker that needs specific accountability structures?⁸ Third, does it require AI-specific regulatory intervention in the context of post-market surveillance in drugs approval or post-market?⁹

The study conducts a doctrinal legal analysis in its methodology approach of analysis of statutory provisions, the judicial principle and regulatory standards applied when considering pharmaceuticals and medical technologies. This is supplemented by a relative regulatory overview of emerging AI governance frameworks of healthcare, especially in technologically

⁴ Frank Pasquale, *The Black Box Society: The Secret Algorithms That Control Money and Information* (Harvard University Press, Cambridge, 2015).

⁵ Richard Goldberg, "Causation and Risk in Pharmaceutical Liability" (2014) 30 *Oxford Journal of Legal Studies* 167.

⁶ European Commission, *Report on the Safety and Liability Implications of Artificial Intelligence* (Brussels, 2020).

⁷ Geraint Howells, "Product Liability and Artificial Intelligence" (2020) 36 *Computer Law & Security Review* 105.

⁸ Ugo Pagallo, *The Laws of Robots: Crimes, Contracts, and Torts* (Springer, Dordrecht, 2013).

⁹ European Parliament, *Resolution on a Civil Liability Regime for Artificial Intelligence* (2020/2014(INL)).

developed jurisdictions. Lastly, this paper has adopted a policy-focused legal critique to assess the normative sufficiency of current models as well as recommend reforms to secure accountability and patient safety and building trust in the operation without impeding innovation.

2. AI in Drug Discovery: Technology, Actors, and Decision Chains

The insertion of Artificial Intelligence in drug discovery has essentially changed the technological framework and the institutional design of pharmaceutical research. The importance of making scientific decisions is primarily human and experimentally verified with a conventional drug development process; in contrast, AI-based drug discovery is based on algorithmic prediction, pattern recognition, and probabilistic inferences on large datasets (UN par. 2). This shift has legal implications in the sense that it redefines the form in which decisions are made, decision makers as well as responsibility in case performance is found to be detrimental.

2.1 Drug discovery AI systems are applied in the field of drug discovery.

Early-stage molecular screening applications that have made broad use of machine learning systems are reviewed by processing large chemical libraries through algorithms that identify the compounds with the greatest likelihood of biological activity. Such systems are based on historical data and keep improving their predictive ability continuously, often without human intervention or proper instructions at any given point. Toxicity, side effects, and drug-drug interaction prediction involve deep learning models, especially neural networks, to identify the non-linear interactions in biomedical data that are complex and difficult to capture through deterministic models without the use of neural networks in their prediction.¹⁰ Although they enhance efficiency, this kind of system is providing a fair deal of uncertainty as far as traceability of decision-making process is concerned since the products of these systems cannot be readily attributed in terms that can be understood by human beings.

Generative AI models are yet another break away of traditional approaches by creating new molecular structures on their own, which could not have previously existed naturally¹¹. They

¹⁰ E. Topol, *Deep Medicine: How Artificial Intelligence Can Make Healthcare Human Again* (Basic Books, New York, 2019).

¹¹ Benjamin Sanchez-Lengeling & Alán Aspuru-Guzik, "Inverse Molecular Design Using Machine Learning" (2018) 361 *Science* 360.

are systems that do not just support the optimisation of existing compounds, but actively form new chemical entities, and this is problematising authorship, foreseeability, and control. Simultaneously, with the increasing application of AI-guided clinical trial simulations, simulation models are being applied to predict trial results, simulate patient response, as well as optimise trial design with artificial control arm and algorithmic patient placement.¹² even mistakes or bias used at this level can have ripple effects impacting decisions of regulatory approval, post-market safety outcomes.

Legally, the technologies erode the difference between decision-support systems and autonomous systems of making decisions. Once AI-based predictions are used to make key safety and efficacy conclusions, the degree of meaningful human supervision turns into a problem of controversy.¹³

2.2 Crucial Stakeholders of AI-Driven Drug Discovery.

The drug discovery ecosystem is a complex web of actors, which are involved in various parts of the decision-making chain and are AI-driven. The pharmaceutical industry is still the main force that develops drugs and introduces them to the market, yet, using secondary AI solutions, the industry is reshaped to an extent that its roles have never resembled before in the historical context of the industry.¹⁴ The algorithms creating the predictions are created and serviced by AI developers and software vendors who usually decline to accept responsibility under contractual restrictions and intellectual property rights.

Another important group of stakeholders is the data providers, who provide the datasets to train AI-based models. The predictive performance of the datasets directly depends on the quality, representativeness, and bias of these datasets but the data providers are often not subject to the standards of pharmaceutical liability due to the limitations of these datasets.[8]. Clinical scientists and contract research organisations use AI outputs in the laboratory and trial environments and invoke different amounts of discretion and validation.

The regulatory authorities serve the role of gatekeepers regarding drug approval and post-

¹² U.S. Food and Drug Administration, *Artificial Intelligence and Machine Learning in Software as a Medical Device* (Discussion Paper, 2019).

¹³ Frank Pasquale, *The Black Box Society: The Secret Algorithms That Control Money and Information* (Harvard University Press, Cambridge, 2015).

¹⁴ Richard Goldberg, "Causation and Risk in Pharmaceutical Liability" (2014) 30 *Oxford Journal of Legal Studies* 167.

market surveillance, however, the prevailing regulatory frameworks were designed based on the human-oriented research methodologies.¹⁵ The proprietary algorithms or training data are often not accessible to regulators, putting a limit on their capability of an independent evaluation of AI-driven decision-making. The many actors in the game make it more difficult to hold a legal accountable because the type of harm could come in as a result of the aggregate of decisions made by various players at various points of jurisdiction.

2.3 Decision-Making Complexity and Legal Implication.

The obscurity of black-box models is one of the greatest challenges presented by the AI-powered drug discovery. A lot of sophisticated AI systems cannot be explained as to the rationale of their output, and it is hard to know why a specific compound has been chosen or why particular safety hazards were underexplained.¹⁶ This inexplainsability negates the conventional rules of law in the standard of proof, which depend on provable arguments and links of causation.

The problem of human-AI collaboration dilemma also makes accountability more difficult. Although humans are officially still in the loop, their contribution can be demoted to accepting or following AI-generated suggestions even when they do not comprehend their foundation properly.¹⁷ This adds confusion on the issue of blame on the human decision-maker or the AI system or the designing or deploying party.

In addition to this, drug discovery through AI also implies distributed responsibility because of the presence of numerous steps and actors. Not one specific defeat can cause harm but the combination of biased information, defective algorithms, and insufficient control.¹⁸ Under these circumstances, it becomes extremely hard to apply the usual tort or product liability principles to assign blame and culpability.

These complexities are of legal relevance in respect of the possibility of lack of effectiveness of the current liability frameworks in offering beneficial solutions. Lack of explicability leads

¹⁵ European Commission, *Report on the Safety and Liability Implications of Artificial Intelligence* (Brussels, 2020).

¹⁶ Geraint Howells, "Product Liability and Artificial Intelligence" (2020) 36 *Computer Law & Security Review* 105.

¹⁷ Ugo Pagallo, *The Laws of Robots: Crimes, Contracts, and Torts* (Springer, Dordrecht, 2013).

¹⁸ Michael Faure & Nils Philipsen, "Liability for Emerging Technologies" (2018) 31 *Journal of European Tort Law* 271.

to conditioning of judicial review whereas the thorny nature of fragmented decision-making creates a problem of responsibility allocation. Consequently, the drug discovery process carried out via AI reveals structural inefficiencies in existing legal frameworks, where a conceptualisation of causation, fault, and responsibility is required to be re-evaluated through the mediation of technologies in the pharmaceutical innovation process.

3. Liability Challenges in AI-Driven Drug Discovery

The application of Artificial Intelligence in drug discovery reveals underlying friction in the current liability models, which have a long-standing history of being constructed on human agency, foreseeability and fault. The assumptions are broken by the AI-powered systems that introduce the concepts of autonomous learning, probabilistic decision-making, and shared responsibility among the actors. Consequently, conventional liability principles, such as product liability, negligence, and vicarious liability, find it challenging to answer logically when a person suffers after innovation with the aid of AI upheld pharmaceutical protection.

3.1 Product Liability

The application of product liability law is based on the fact that there exists a material or recognisable product which is either defective in design, production, or warnings. When it comes to the AI-driven drug discovery, the initial problem is whether an AI-generated drug, or the AI itself that was used to create this drug, will be deemed as a product at all. The ultimate pharmaceutical compound is, surely, a product, but the damage can be caused by the decisions made by the algorithm long before the manufacturing process starts.

The issue of the attribution of defects is especially troublesome in the case of the autozoetic learning of the algorithm. The predictive models are continuously updated with new information as machine learning systems go, so the behaviour of the system at the time of harm might not be the same as it was at the time of deployment.¹⁹ This dynamic development contradicts the old concept of a fixed defect at a point of sale. Courts will struggle to know whether a fault is in the original design, the training data or the autonomous learning process that followed therewith.

¹⁹ European Commission, *Report on the Safety and Liability Implications of Artificial Intelligence* (Brussels, 2020).

Bias in data also makes defect analysis difficult. In case AI system is trained on non-representative or biased data, its prognostications on the matters of safety, dose or efficacy can be inherently faulty.²⁰ Nevertheless, this bias might not be so overtly exhibited and only visible later via adverse reactions to the drug after approval. The designation of the responsibility in these situations begs the question of whether the fault is in the AI system or the given data or the inability of the pharmaceutical company to identify or resolve these limitations. The current product liability regime systems provide little assistance on assigning the blame on harms that are based on the inference of data that are not based on physical faults and defects of a product.²¹

3.2 Negligence and Standard of Care.

Legality The negligence needs to be shown to have a duty of care, breach, cause and damage. The use of AI in drug discovery creates a major doctrinal dilemma in defining the relevant standard of care. Pharmaceutical companies are traditionally required to conduct reasonably in the conduct of research and testing, and conscientiousness in regards to regulation. The entry of AI into the picture makes this criterion more complicated as it draws issues regarding what is considered a reasonable use of the algorithmic recommendations or not.²²

A major concern is that AI as a concept raises or decreases the anticipated standard of care. On the one hand, AI systems can be considered futuristic technologies, which will make the process of predictions more accurate and thus increase the standards of safety and diligence. Conversely, their obscurity and incomprehension can warrant some form of submission to the outputs of the algorithms especially when the experts in the field do not have the ability to verify forecasts on their own²³.

The crisis of human dependence on AI recommendations is the main issue of the study of negligence. The over-reliance can happen because human researchers do not question AI outputs adequately, thus leaving exceptionally important safety decisions to machines. On the

²⁰ Sandra Wachter, Brent Mittelstadt & Luciano Floridi, "Why a Right to Explanation of Automated Decision-Making Does Not Exist in the GDPR" (2017) 7 *International Data Privacy Law* 76.

²¹ Richard Goldberg, "Causation and Risk in Pharmaceutical Liability" (2014) 30 *Oxford Journal of Legal Studies* 167.

²² U.S. Food and Drug Administration, *Artificial Intelligence and Machine Learning in Software as a Medical Device* (Discussion Paper, 2019).

²³ Frank Pasquale, *The Black Box Society: The Secret Algorithms That Control Money and Information* (Harvard University Press, Cambridge, 2015).

other hand, an under supervision can occur when humans do not have the technical skills needed to supervise AI systems in any meaningful sense and hence, supervision is formal but not substantive. Using the theory of blame, it is hard to pinpoint blame in either of the two cases, because not only do human actors respond in line with what is being practiced within the industry, but also are part of the negative results.

There is another challenge of causation. It is almost hard to prove a direct causal relationship between a particular AI-based prediction and resulting patient harm, especially when numerous steps of decision-making are involved between them.²⁴ Consequently, negligence claims subject to being defeated on grounds of evidence gaps instead of being unjustified.

3.3 Vicarious and Shared Liability.

The vicarious liability has conventionally made it possible to hold the employers or principals liable on behalf of the actions of their agents. However, in the field of AI-based drug discovery, AI systems do not conveniently fall under the legal definition of an agent since the systems do not possess legal personality and intent.²⁵ The agency that could be able to hold pharmaceutical companies responsible of the implementation of AI tools would be a simplistic approach that is likely to ignore the fact that the interdependence between pharma companies and AI developers is complicated.

In the design of the system, model structure and training processes, AI developers as well as software vendors often determine system behaviour. However, contractual dealings often contain clauses that spread the risks that involve transferring of risks, which capped or exempted the developers of the contractor.²⁶ This type of contractual constraint might not serve the purpose of patient or consumer protection especially in the cases where the interests of the populace necessitate responsibility beyond the confines of individual requesting.

The distributed responsibility has been addressed through the idea of shared or joint liability. Within these kinds of models, pharmaceutical companies, AI developers, and other stakeholders would share responsibility and be liable as well as severally to harm caused by

²⁴ David G. Owen, "Products Liability: User Misconduct Defences" (2019) 52 *South Texas Law Review* 1.

²⁵ Lawrence B. Solum, "Legal Personhood for Artificial Intelligences" (1992) 70 *North Carolina Law Review* 1231.

²⁶ Christopher Hodges, *Law and Corporate Behaviour* (Hart Publishing, Oxford, 2015).

AI-assisted drug discovery.²⁷ Although this solution increases victim compensation, it brings with it the issues of fairness, deterrence of innovation and proportionality to the case particularly when actors within the game have unequal amounts of power.

The essence of all these issues of liability is that the traditional liability which is based on fault assumes human intent, knowledge, and control. With AI-driven drug discovery, the harm might happen with no knowable human malpractice, but rather due to greater system behaviour or to intricate interactions among data and algorithms as well as human choices.²⁸ This contrast between the legal theory and technological facile highlights how balancing liability distribution in safety critical AI applications should be redone..

4. Accountability and Governance Deficits in AI-Driven Drug Discovery

The application of a trial of Artificial Intelligence to drug discovery demonstrates profound governance and lack of accountability that current frameworks of laws cannot address. In contrast to traditional pharmaceutical research, where human actors can be tracked through the lines of decision-making authority and responsibility, in AI-driven processes, the decision making is handled via opaque systems, fragmented institutionality and intriguing technological dependencies.²⁹ All these characteristics work against the assigning of the blame, regulatory control, and the validity of AI-based medical innovation.

4.1 Accountability Gaps

One of the main areas of accountability is lack of legal personality of AI systems. AI-based drug discovery researchers lack legal personality and do not have a rights and liability, but offer services that have a material impact on safety-related decisions.³⁰ In the situation when negative consequences take place, liability should hence be redirected towards human or corporate actors, despite the lack of any individual actor having a direct control of the harmful decision. This generates an institutional discrepancy between responsibility and causality.

²⁷ European Parliament, *Resolution on a Civil Liability Regime for Artificial Intelligence* (2020/2014(INL)).

²⁸ Andreas Renda, "Artificial Intelligence and Liability: What Should the EU Do?" (2021) 13 *Journal of European Tort Law* 1.

²⁹ World Health Organization, *Ethics and Governance of Artificial Intelligence for Health* (WHO, Geneva, 2021).

³⁰ Lawrence B. Solum, "Legal Personhood for Artificial Intelligences" (1992) 70 *North Carolina Law Review* 1231.

The fact that the logic behind making these decisions is not traceable is also worsening the problem. Most AI systems are black systems, which give outputs without any sensible explanations.³¹ This obscurity in drug discovery has made it impossible to regulators, courts, and even pharmaceutical companies themselves to tell why this compound or that one was favoured, risks underestimated, or patients ruled out. In the absence of traceability, review, audit and justification mechanisms of accountability would be useless.

Accountability is further watered down in supply chains involving complex supply chain. Many actors are typically involved in AI-driven drug discovery: data providers who provide training datasets, AI designers who create algorithms, pharmaceutical firms who implement the outputs and regulators who accept the final products. The harm can be the result of such interaction of the decisions being made at various stages in this chain, and not due to a single failure. The systems of traditional laws where linear causation is the basis and an individual is guilty find the responsibility in such distributed surroundings very difficult to ascertain.

4.2 Explainability and Transparency.

Explainability has become a foundation of accountability in AI governance especially in risky areas like healthcare. Explainable AI (XAI) is a grouping of systems able to offer some light into the manner and reason behind the development of certain outputs. Regarding drug discovery, explainability goes beyond being a preference in the technical sense, but a legal requirement as well. Regulatory approval, judicial review and post market surveillance all require one to be able to evaluate the rationale behind safety and efficacy decisions.

Litigation presents a serious evidentiary problem due to the lack of explainability. Claimants who want redress because of harm inflicted by AI might not be able to prove the causation or breach of duty unless the algorithmic reasoning or training data is available.³² Courts which are used to weigh the evidence of the experts and documents will not be able to appraise the decision of algorithms, which is based on algorithms and will not receive any significant attention. This may result in depriving of good remedies and may render the liability law useless in its deterrent role.

³¹ Frank Pasquale, *The Black Box Society: The Secret Algorithms That Control Money and Information* (Harvard University Press, Cambridge, 2015).

³² Richard Goldberg, "Causation and Risk in Pharmaceutical Liability" (2014) 30 *Oxford Journal of Legal Studies* 167.

Also, there exist tension between transparency and protection against intellectual property. The creators of AI algorithms are often claimers of such trade secrecy due to the ideas with pharmaceutical firms, and many of these models.³³ Although these protection mechanisms may help to encourage innovation, over-secrecy may hamper regulatory and public health responsibility. When it comes to drug discovery, as the decisions made have a direct impact on patient safety, the lack of balance between the interests of the proprietors and the disclosure problems becomes a very sensitive issue. There is a danger that the inability to balance these conflicting interests could destroy trust in AI-based medicines among people.

The fourth principle is ethical accountability and public trust, which involves demonstrating honesty and trustworthiness to those around them.

4.3 Ethical Accountability and Public Trust

The fourth principle is ethical accountability and public trust, which entails being truthful and trustworthy to the people around them.

More than the issue of formal accountability in law, AI-assisted drug discovery presents some very compelling ethical issues that directly touch on the legitimacy of governance. One of the risks that will persist regardless of the method employed is algorithmic bias, and this risk is likely to occur especially when the training data does not adequately represent some people in relation to their ethnicity, gender, age, or geographical location.³⁴ Inequalities in health caused by biased datasets may create less effective and more harmful drugs to marginalised populations, creating new health disparities.

There are also chances that discriminatory results in AI-assisted clinical trials will emerge. The patient selection and stratification tools, driven by AI, can omit some of the groups, which are considered statistically, the least optimal, even in situations when this omission is not an ethically justifiable objective. These customs contravene such core values of medical ethics as equity, inclusiveness, and respect of a person.

The element of public trust is an extremely important and delicate aspect of pharmaceutical governance. Drugs created via inexplicable and opaque AI algorithms will be questioned by people, especially in case of some adverse events without explanations or responsibility.³⁵ Efficiency does not even maintain trust but rather transparency, fairness, and the guarantee that the human values are not lost in technology decision-making. AI-based drug discovery lacks accountability and governance frameworks, which compromise its credibility in the long run in society.

5. Regulatory Frameworks: National and Comparative Perspectives

AI-driven drug discovery is regulated at the boundary between the pharmaceutical regulation and the novel AI regulation. Nonetheless, they have developed to a great extent in seclusion, leading to regulatory blind spots in which algorithmic decision-making takes a decisive part in the drug development process.³⁶ In this section, the existing pharmaceutical regulations frameworks, emerging models of AI specific and comparative models with jurisdictions are critically asked, which means that an integrated regulatory architecture will be necessary.

5.1 Pharmaceutical Officer- Pharmaceutical regulation is effective in Thailand.

Regimes that are used to approve drugs globally are based on scientific research, clinical trials, and regulatory inspection led by human beings. Safety, efficacy and quality are usually evaluated by regulatory authorities using pre-established test stages, and proficient judgment of safety, efficacy and quality.³⁷ Although these regimes guarantee a high standard of questioning, they do not plan on questioning algorithmic decision making processes in drug discovery.

A major blind spot is the fact that regulators are not able to evaluate AI-based predictions applied in identifying targets, screening of toxicity, or designing trials. The submissions made to the regulators are usually concerned with the experimental results and not the computing routine that informed the results. Consequently, AI systems that make critical safety decisions are left unregulated in most cases.

There are also weaknesses in the post-market surveillance systems to deal with AI risks. The pharmacovigilance models are based on adverse events reporting and statistical surveillance, which can not identify the harmful results of biased algorithms or incorrect predictive models until significant amounts of damage have been inflicted by them on a large scale.³⁸ Besides, AI systems are not generally made available to regulatory bodies even after they have been approved, and regulators are therefore constrained in their ability to act upon changing

³⁶ World Health Organization, *Ethics and Governance of Artificial Intelligence for Health* (WHO, Geneva, 2021).

³⁷ Joseph A. DiMasi, Henry G. Grabowski & Ronald W. Hansen, "Innovation in the Pharmaceutical Industry: New Estimates of R&D Costs" (2016) 47 *Journal of Health Economics* 20.

³⁸ Richard Goldberg, "Causation and Risk in Pharmaceutical Liability" (2014) 30 *Oxford Journal of Legal Studies* 167.

algorithmic behaviour.

5.2 Specific AI Regulatory Models.

Due to the weaknesses of conventional regimes, AI-specific regulatory models have shifted towards a risk approach more frequently. Within this model, the AI systems are controlled based on the degree of damage that they can disrupt with healthcare and pharmaceutical opportunities being the high-risk category of applications. This strategy acknowledges that the application of AI in the discovery of drugs requires a higher level of scrutiny since it directly affects the health of people.

As a popular regulatory tool, pre-market AI validation has appeared. Some of the validation requirements can be testing the performance of the algorithms used, testing the quality of training data, and others checking against bias and error. In contrast to traditional software approval, AI approval has to consider adaptive learning and probabilistic results, which presents complicated questions concerning what percent of uncertainty is acceptable.

Obligations to provide permanent monitoring should also be seen as another important characteristic of AI-specific regulation. Since AI systems can advance after implementation, regulators are placing more importance on lifecycle management, such as regular audits, performance reporting, and updates, as mandatory.³⁹ These commitments are supposed to avert regulatory obsolescence and also make sure that safety standards are abreast with technological change.

5.3 Competitive Regulatory styles.

One of the most widespread methods of regulation of AI has been implemented in the European Union, where AI systems in the health care field are classified as high-risk. Medical systems based on AI should be strictly assessed for conformity, have a transparency requirement, and be supervised after implementation in-market under this framework.⁴⁰ This strategy specifically identifies the systemic risks of AI and aims to introduce responsibility across the lifecycle of AI implementation.

³⁹ Andreas Renda, "Artificial Intelligence and Liability: What Should the EU Do?" (2021) 13 *Journal of European Tort Law* 1.

⁴⁰ European Parliament, *Resolution on a Civil Liability Regime for Artificial Intelligence* (2020/2014(INL)).

Conversely, the United States is a sectoral and agency based model. In drug discovery, the primary way that AI is regulated is through the Food and Drug Administration where a guideline is issued instead of an AI-specific law.⁴¹ On the one hand, this flexible solution contributes to innovation, but on the other hand, there is a risk of regulation fragmentation, unequal oversight, especially in cases when AI functions go beyond the boundaries of traditional medical devices.

Jurisdictions in development are also more and more taking up AI governance, but regulation frameworks are still in an early form. Most of them depend on generic pharmaceutical policies that are complemented by soft-law AI policies.⁴² Although this model will lower compliance costs in the short-term, it can make populations susceptible to unregulated algorithmic dangers, especially in cases where regulatory capacity is low.

Criticism is a fundamental cornerstone of the research.

The other weakness that is reviewed over and over again between jurisdictions is the division between AI law and drug law. Pharmaceutical authorities tend not to have the technical requirement to, and AI regulators might not be domain-related expertise in the safety of drugs.⁴³ This separation introduces responsibility gaps in which the decisions made by AI have an impact and are not fully monitored.

The complexity of having an integrated regulatory architecture is thus urgent. This would place AI governance into the context of the pharmaceutical regulation, where transparency of algorithms, validation, and monitoring should be regarded as the essential facets of drug safety. In the absence of integration in regulation, AI-based drug discovery will run ahead of the regulations and will compromise patient safety and trust.

6. Way Forward: Legal Reforms and Policy Recommendations

The above discussion shows that AI-led drug discovery reveals the systemic failures of the current liability and regulatory regulations. These deficiencies are not just a result of regulatory

⁴¹ U.S. Food and Drug Administration, *Proposed Regulatory Framework for Modifications to Artificial Intelligence/Machine Learning-Based Software as a Medical Device* (2021).

⁴² Organisation for Economic Co-operation and Development, *Artificial Intelligence in Society* (OECD Publishing, Paris, 2019).

⁴³ Michael Faure & Nils Philipsen, "Liability for Emerging Technologies" (2018) 31 *Journal of European Tort Law* 271.

inertia, but reflect more fundamentally a conceptual lack of fit between legal principles as human centric and technological decision making being technology centric. The section will contain legal and policy proposals to ensure accountability is restored, patient safety and innovation is maintained in the pharmaceutical research.

6.1 Reconsidering Liability Models.

The conventional fault-based liability regimes find it difficult to resolve the harm that may be caused by AI-guided drug discovery as the harm may be caused without any specific human mistake or intent. Strict liability of high-risk AI drug systems is one of the possible reforms in this direction. With a strict liability regime, pharmaceutical firms using AI in safety critical phases of drug discovery would be liable to the harm caused regardless of fault.⁴⁴ This practice is in line with the set principles in the jurisprudence on hazardous activities, such that the safety of the people is paramount compared to the requirement to establish negligence.

Strict liability is more reasonable when AI systems form independent systems, they learn and make decisions that directly impact human health. Incentivising pharmaceutical firms to implement strong validation, monitoring, and risk-reduction procedures by internalising the costs of risk, such a regime increases the likelihood of compliance with these policies (Levin 2010, p. 106). Nevertheless, the scenario may hinge on strict liability may relocate disproportionate liability to the end-users of AI, especially where the harm is linked to the algorithmic design or the data bias.

To accommodate this unequal situation, there is need to implement mandatory insurance schemes when it comes to pharmaceutical research that is assisted by AI. Compulsory insurance would also cover the damages to the victims even when the cause of the elevated risk to those insured is hard to determine and spreads the risk among those insuring and the industry players. These plans have a history of application in environmental liability and medical malpractice cases and can become a viable risk-sharing instrument.

Besides, shared liability models provide a more just distribution of responsibility among the players in AI-based drug discovery. Attributing to this model, lawsuit can be held jointly and severally against pharmaceutical companies, developers of AI and data providers, and internal

⁴⁴ Michael Faure & Nils Philipsen, "Liability for Emerging Technologies" (2018) 31 *Journal of European Tort Law* 271.

contribution mechanisms are applicable.⁴⁵ Although such a method poses the issue of innovations being discouraged, it is a characteristic of the distributed decisions and avoidance of the element of accountability in contractual fragmentation.

6.2 Regulatory Reforms

Regulatory restructuring should accompany the liability reform. Regulatory frameworks in place need to include AI-particular layers of approval that need to be disclosed and evaluated AI systems deployed during drug discovery. These layers would require a record of the purpose of the algorithm, the nature of training data, the metrics of validation and the results of limitations that are known to exist.⁴⁶ This would enable the regulators to evaluate the outcomes as well as the processes that determine it.

The safety-critical AI requires explainability requirements. Regulations officials must demand that AI applications to drug discovery to have adequate explainability thresholds, so they may be under meaningful human control and can be investigated after harm occurs.⁴⁷ Complete transparency cannot be technically practiced, but functional explainability (to evaluate risk and accountability) should be considered as an obligatory feature but not as an optional one.

Regulatory sandboxes present a viable mechanism of balancing between innovation and regulation. Sandboxes would allow regulators to gain insight into the dangers of technology and developers to have legal security by allowing them to conduct controlled testing of AI-assisted drug discovery under regulation oversight. Dynamical rule-making grounded on empirical experience and not speculative risk evaluation is also enabled by such mechanisms.

6.3 Conclusion

The use of AI-based drug discovery can not be regulated like a neutral software or even a routine research infrastructure. The way it can decide on matters affecting safety on its own puts it in a class of technologies that require greater legal accountability. The myth that AI is a tool hides the fact of system causality and the responsibility.

⁴⁵ European Parliament, *Resolution on a Civil Liability Regime for Artificial Intelligence* (2020/2014(INL)).

⁴⁶ European Commission, *Report on the Safety and Liability Implications of Artificial Intelligence* (Brussels, 2020).

⁴⁷ Sandra Wachter, Brent Mittelstadt & Chris Russell, "Counterfactual Explanations without Opening the Black Box" (2018) 31 *Harvard Journal of Law & Technology* 841.

As the field that has a direct impact on human life and the state of health, drug discovery needs the framework that functions under prioritisation of safety, transparency, and trust. This requires the transformation of human-oriented accountability, which is based on individual blame, to the system-oriented accountability, which is in a position to respond to distributed decision-making and emergent technological behaviour.⁴⁸

The evolution of the law is not needed to oppose AI advancement, but to ensure it is punished. In the absence of coherent models of liability and governance structure with combined regulations, AI-based drug discovery would damage the trust of the people and subject patients to risks that are impossible to control. An alternative legal system that is based on responsibility, explainability, and precaution provides the best long-term future of technologically mediated pharmaceutical innovation.

⁴⁸ World Health Organization, *Ethics and Governance of Artificial Intelligence for Health* (WHO, Geneva, 2021).