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Explainable Artificial Intelligence as a Legal Tool for AI-Assisted Pharmaceutical Patents: Lessening the Black-Box Problem Under 35 U.S.C. § 112

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Abstract: The rapid integration of artificial intelligence (AI) into pharmaceutical research has accelerated drug discovery, but the opaque, "black-box" nature of deep learning models creates severe legal hurdles under 35 U.S.C. § 112. Because inventors often cannot explain how complex algorithms reach specific molecular predictions, AI-assisted patent applications risk rejection for failing to satisfy statutory written description and enablement requirements. Inventors are further constrained by the dilemma of either publicly disclosing proprietary source code or foregoing patent protection entirely. This paper examines whether Explainable Artificial Intelligence (XAI)—utilizing methods such as LIME and SHAP—can serve as a legally sufficient tool to mitigate this dilemma. By translating opaque computational decision-making into interpretable feature attributions and transparent reasoning pathways, XAI allows applicants to demonstrate possession and enable a person having ordinary skill in the art (PHOSITA) without compromising trade secrets. Although explainability cannot bypass core requirements like patent eligibility, novelty, or non-obviousness, it provides a practical evidentiary bridge that aligns AI-driven drug development with the public-disclosure bargain foundational to patent law.

Keywords: Explainable Artificial Intelligence (XAI), 35 U.S.C. § 112, Patent Enablement, Black-Box Problem, AI-Assisted Drug Discovery, Pharmaceutical Patents

I INTRODUCTION

A. BACKGROUND

In recent years, there has been rapid growth in the use of Artificial Intelligence (AI) within the healthcare industry, including applications such as treatment planning and drug discovery [1]. This development stands to revolutionize the industry, promising to significantly shorten the lengthy path from molecular discovery to market approval [2]. Currently, drug discovery typically involves targeting a protein implicated in a disease and developing a compound that binds to it and modifies its activity [3]. Artificial intelligence can conduct large-scale simulations, analyze vast amounts of health research data, and utilize generative chemistry to design new molecules based on protein structures [4]. Prior achievements in molecular identification and interaction have shown the potential of to accelerate the pharmaceutical research and development process [5]. However, the increasing advancement and sophistication of AI within drug development creates considerable regulatory challenges for inventors seeking to claim a patent [6].

Under 35 U.S.C. § 112(a) patent applications must contain a clear written description of the invention that allows a person having ordinary skill in the art (PHOSITA) to make and use the invention without undue experimentation and must disclose the best way to use the invention [7]. Patent claims must also explicitly define the inventions under 35 U.S.C. § 112(b), while functional claiming is governed by Under 35 U.S.C. § 112(f) [8]. In recent years, Congress has recognized that patents may be granted for certain inventions created with the use of artificial intelligence, on condition that the existing requirements of inventorship are met [9].

Additionally, the United States Patent and Trademark Office (USPTO) in its 2024 *Inventorship Guidance for AI-Assisted Inventions*, stated that a patent could be issued if one could prove that a human individual "significantly contributed" to the invention [10]. Later, the *Revised Inventorship Guidance for AI-Assisted Inventions* in 2025 reinforced that AI models cannot qualify as an inventor. Rather, AI is treated as a research tool, requiring that the human inventor demonstrate a significant contribution to the development of the claimed invention [11].

Artificial Intelligence often functions as a "black box," where its internal decision-making processes can be opaque [12]. This is a significant issue, as it poses a difficulty in fulfilling the disclosure requirements of U.S.C. § 112, which requires that an invention be described in sufficient detail to enable a skilled individual to recreate it without undue experimentation [13]. For developers, this can be concerning as they must disclose their methodology. Explaining specific model architectures or training data raises the risk of exposing their proprietary technology to competitors [14]. A growing research topic has emerged that could mitigate this issue. Using Explainable Artificial Intelligence (XAI), a branch of machine learning, it aims to *untangle* AI systems' "black box" reasoning [15]. Rather than treating the AI outputs as opaque, XAI seeks to identify, visualize, and explain the internal logic that leads to predictions and conclusions [15].

B. Thesis

To date, neither Congress nor the courts has specifically addressed whether Explainable Artificial Intelligence may help satisfy the written description and enablement requirements of 35 U.S.C. § 112 for AI-assisted inventions [9]. However, the existing patent doctrine suggests that XAI has the potential to mitigate the legal uncertainties posed by "black-box" AI-assisted inventions by making the invention process more transparent and interpretable. Subsequently, XAI may strengthen patent applications by demonstrating possession of the invention, supporting the written description and enablement requirements under 35 U.S.C. § 112, and providing sufficient disclosure without divulging proprietary algorithms.

C. Questions Examined

This article examines whether Explainable Artificial Intelligence (XAI) should be seen as a legally sufficient tool for mitigating the "black-box" problem in fulfilling the patent disclosure requirements for AI-assisted healthcare inventions.

II. Artificial Intelligence in Healthcare and the "Black Box" Problem

A. Current uses in the healthcare industry

The implementation of artificial intelligence in healthcare can address systemic challenges that have burdened healthcare professionals, such as administrative tasks, the accuracy of medical image interpretation, and the lengthy drug discovery process [1]. Artificial intelligence can model complex biological systems and subsequently identify the most hopeful prospects, thereby accelerating workflow and innovation [3]. By 2022, over 62,000 AI-related patent applications had been granted globally, with many of them encompassing life sciences [2]. Through machine-learning analysis, data integration, compound design, laboratory synthesis, feedback, and testing, AI accelerates compound identification in drug development [3].

A. Deep Learning

Artificial Intelligence currently contains classical programming and machine learning (ML), with ML containing many models and methods—such as deep learning and artificial neural networks [16]. Machine learning is a field of artificial intelligence that focuses on algorithms that analyze large datasets to identify patterns [16]. Compared to classical programming, where an algorithm is explicitly coded as instructions, machine learning uses vast amounts of data to learn an algorithm that, over time, can make decisions, make predictions, or generate content [16]. Although the outputs and inputs of these models are known, their internal workings are largely inaccessible and poorly understood [12]. To describe this phenomenon, the term "black box" is used [12]. This issue can be attributed to several different factors—including the intricate structure of deep learning models and the complexity of their interactions—which make the specific conclusions difficult to trace [15]. Moreover, minute differences in input data can lead to entirely different outputs, making these models entirely unpredictable [12].

B. Legal Implications

35 U.S.C. § 112 requires inventors to provide sufficient disclosure to demonstrate how an invention works and how a person possessing ordinary skill in the art (PHOSITA) can make and use it without undue experimentation [7]. The opaque nature of these "black box" models offers a significant challenge to these disclosure requirements [13]. If an artificial intelligence model's internal logic or algorithm is opaque even to its inventors, patent examiners may deem the applications as legally insufficient because they fail to satisfy the disclosure requirements [13]. Without an adequate explanation of how an AI-assisted invention contributed to its results, replication becomes increasingly difficult, thereby increasing the risk of patent rejection [14].

Additionally, developers frequently are often forced to choose between maintaining AI algorithm code as a trade secret or publicly disclosing it to obtain patent protection [14]. Besides patent law, opaque "black box" models pose a risk to healthcare providers, as the lack of explanations for AI decisions can create liability concerns. If clinicians fail to analyze or understand the conclusions provided by AI, they may be unable to recognize and rectify errors, which can potentially impact patient safety and professional responsibility [17]. This lack of explainability in AI models

poses challenges not only to clinical trust but also to patent law [17].

III. Explainable Artificial Intelligence (XAI)

A. Definition

Explainable Artificial Intelligence (XAI) is a developing field of machine learning that strives to *decode* the opaque internal logic of AI systems, directly combating the "black box" problem [18]. These processes enable human users to understand the results produced by machine learning algorithms, deep learning, and neural networks [12]. Rather than "traditional" artificial intelligence, XAI utilizes specific techniques and methods to ensure that, during the ML process, each decision made can be tracked and explained [15]. However, it is important to note the differences between explainability and interpretability within AI. Explainability describes how the artificial intelligence model arrived at its results, while interpretability concerns the extent to which an outside observer can understand the reasons for the decision [18]. As AI becomes more sophisticated, ML must be understood and monitored to ensure its results are accurate, and XAI provides methods to achieve this [15].

B. Major Methods

Each of the techniques and methods of XAI approaches AI to make complex decisions more understandable. The methods of XAI can be clustered into groups such as transformer-based approaches, activation-based, attribution-based, and perturbation-based [19].

Activation-based methods commonly use feature maps or activation values to weight them according to their importance to the final output, effectively visualizing and interpreting what deep neural networks "see" [20].

Attribution-based methods generate saliency maps—numerical representations that highlight the most important regions in a data input—by tracing the model backward from the prediction to the input. These methods typically rely on either gradients or activations and assume that changes in the model's input that affect its output indicate a feature's importance [21].

Perturbation-based XAI methods aim to explain predictions by directly altering the initial input and observing how the output changes. LIME (Local Interpretable Model-agnostic Explanations) is a specific technique that uses the perturbation process to understand how the model behaves. LIME assigns higher weights to samples that are most similar to the original and lower weights to those that are more distant. Using these weights, a simple, interpretable model is built, and its coefficients indicate the importance of each feature for that specific prediction [22].

Similarly, SHAP (SHapley Additive exPlanations) assigns scores that reflect fair "contributions" to each feature by evaluating all possible combinations of features. Unlike LIME, SHAP is based on cooperative game theory to guarantee consistency and theoretical fairness [23]. Transformer-based models use the attention mechanism, often with attention weights or attention rollout techniques, to create visual explanations [19].

C. Advantages

These methods enable prediction accuracy and traceability, with the former focusing on technological requirements and the latter on human needs. By generating simulations and comparing XAI outputs with results from the training set, users can determine prediction accuracy [19]. Using methods like SHAP, where values are given to show which feature provided the most contribution to the output, clinicians can validate results against their clinical training and identify where the model may be misled or overlook data [23]. Therefore, this would reduce the harm caused by flawed outputs and increase interpretability [24]. By *breaking down* how input data is processed, observers would be able to understand exactly what the model is doing—improving the transparency of the AI model's inner workings and ensuring it is documented [19]. XAI can also improve audibility by enabling the tracing and evaluation of model behavior, allowing internal users and external regulators to understand why errors occurred [25] and possibly allow for compliance with legal requirements such as privacy laws and 35 U.S.C. § 112.

IV Patent Law Framework for AI-Assisted Drug Development

A. Purpose of patent Law and Pharmaceutical Innovation

Patent law was established to encourage scientific and technological innovation within the United States to drive economic growth [26]. Currently, Title 35 of the U.S. Code sets forth the statutory principles governing patent law. Designed to spur innovation, patent ownership grants a short-term monopoly over the use of an invention in exchange for public disclosure. Rather than securing an inventor's natural rights in their discoveries, a patent is a reward intended to promote progress and knowledge [27]. The hope was that this would enable the public to use the disclosed technical details to engage in innovative activities later [13].

In pharmaceutical research, they grant an inventor exclusive rights to manufacture, use, and sell a particular drug or product—protecting its chemical structure, manufacturing process, or active use [28]. This incentive theory can be understood in the context of high costs of pharmaceutical development, testing, and regulation. These patents are

deemed necessary to allow pharmaceutical manufacturers to recoup the costs of research and development and last approximately 20 years [29]. However, much of this time is lost to the lengthy U.S. Food and Drug Administration (FDA) review and clinical testing phases, which can account for roughly half of the patent term [29]. Currently, there is an abundance of compounds available to pharmaceutical companies that can potentially combat numerous specific diseases; however, these companies lack the appropriate tools for the compounds [30].

With the utilization of Artificial Intelligence, the drug discovery and clinical development process is being reshaped through compressed discovery timelines and improved success rates [2]. AI-assisted Algorithms can analyze large datasets to rapidly predict the efficiency of specific drug candidates and identify potential targets [31]. Berg, a Boston-based biotech company, has developed an AI-assisted platform that contains a large patient database and is used to identify and validate the specific biomarkers responsible for diseases, and to decide on appropriate treatments. The company's motto is to compress the lengthy drug discovery process and reduce overall costs by implementing AI, which reduces guesswork [31]. Alpier et al. presented the first successful approach to using deep neural networks (DNNs) to predict pharmacological activities across numerous drugs [31]. AI-assisted tools have also been used to predict the toxicity of drug molecules to avoid harmful effects [3].

Patent protection remains essential for these AI-driven research and development projects because companies require meaningful intellectual property protection to justify the substantial financial costs associated with A—driven drug development. For decades, the industry has argued for increasing protections against data exclusivity, rising costs, and risks for the development of new drugs [32].

A. Eligibility

35 U.S.C. § 101 governs patentable subject matter and defines what constitutes a patent claim in the United States. The statute states, "whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title" [33]. § 101 establishes four primary categories of subject matter that are eligible for a patent: processes, machines, manufactures, and compositions of matter [33]. To prevent a monopoly and the stagnation of innovation, the Supreme Court has expressed concern over granting patents involving abstract ideas, laws of nature, and natural phenomena through the Manual of Patent Examining Produce (MPEP § 2106) [34]. 35 U.S.C. § 102 is the statute that defines "novelty" and "prior art." It describes that an invention must be completely new and distinct, and that a patent will not be granted if the claimed invention was previously known, used, published, patented, or sold prior to the filing date [35]. The "non-obviousness" requirement is governed by 35 U.S.C. § 103. It states that a patent cannot be granted if a claimed invention's differences from prior art would have been obvious to a person having ordinary skill in the art (PHOSITA) before the filing date. The modern framework for evaluating non-obviousness was established by the Supreme Court in Graham v. John Deere Co., which continues to be the ruling precedent for obviousness determinations [33]. The use of AI within claimed inventions involving drug developments does not conflict with these statutes; however, U.S.C. § 112(a) constitutes a significant issue [36].

Section 112(a) details the minimum specification requirements for patent applications. It states that an application must include a written description of the invention and disclose sufficient information to enable a PHOSITA to make and use the invention without undue experimentation. Additionally, applicants cannot conceal the best way of practicing the invention from the public [9].

C. The Legal Consequences of the Black Box

The use of AI models and their opaque internal logic causes conflict with patent law. The exact reasoning and explanations for the result are unclear, therefore failing to meet the written description and enablement requirements—patents can be invalidated as a result [13]. This is especially apparent in AI-assisted pharmaceutical inventions, as inventors must explain their inventions thoroughly —a task hindered by the opaque nature of AI, its "black box" problem [13]. This issue is not primarily technical, and "black box" systems challenge the "quid pro quo" of patent law.

V Proposed Legal Applications

By providing sufficient transparency into patent examination, litigation, and commercialization, Explainable AI (XAI) has the potential to reduce legal conflicts associated with black-box algorithms without eliminating the competitive advantages of proprietary AI systems. Rather than requiring disclosure of proprietary code or model architecture, XAI provides an interpretable explanation of how AI tools arrive at their conclusions and recommendations, thereby improving transparency [37].

A. XAI Throughout the Patent Lifecycle

Involving drug discovery, XAI enhances transparency in molecular ML algorithms through prediction, modeling, and design [38]. By using metrics such as fidelity, interpretability, stability, and consistency XAI can clarify the pathways and

explain why specific disease targets were flagged [38]. Additionally, methods such as SHAP or LIME interpret model predictions by showing the specific contribution of each feature, enabling pharmaceutical developers to understand the key factors influencing a compound's predicted activity [39]. XAI addresses the explainability issue by producing clear explanations of model predictions, thereby increasing trust, enabling error detection, and facilitating a higher understanding of model behavior [39].

During the patent examination process, XAI has the potential to assist the USPTO and examiners in verifying that human inventorship requirements are met. XAI allows for the identification of the exact algorithm and modifications that demonstrate a new, non-obvious innovation separate from prior art [9]. It can also assist examiners in determining patent eligibility by separating patentable chemical or structural innovations from non-patentable abstract concepts or laws of nature [37]. Additionally, increased transparency gives stakeholders greater confidence—because XAI provides clear evidence of a drug's probability of success—and reduces the perceived risk of AI-assisted inventions [37]. XAI bridges the prevalent gap between the opaque internal logic of the algorithm and real scientific validation.

VI Theoretical Application

Since this concept is relatively new, this paper discusses a detailed hypothesis to assess the role of XAI in AI-Assisted Drug Patents. Hypothetically, consider a biotechnology company that develops an AI-assisted platform for the initial stages of the drug discovery process. This platform analyzes thousands of potential chemical compounds and identifies the most promising candidate that can be further developed into a new drug. Following the AI platform's recommendations, the biotech company invests substantial resources in laboratory testing and later concludes that the compound has therapeutic potential. The company then creates a patent claim for the newly identified compound and the AI-assisted platform used during the initial discovery process. However, during patent examination, questions are raised regarding the reliability and significance of the AI's contribution. Because the AI's internal decision-making operates as a "black box," the company cannot explain why the model chose this specific compound over thousands of other potential candidates—although it can describe the training data and overall validity [38]. This would subsequently cause the patent claim to fail to fulfill the established requirements of 35 U.S.C. § 112(a), regarding written description and enablement [7].

However, suppose the company employs an Explainable Artificial Intelligence (XAI) model, such as LIME or SHAP. The system can generate an interpretable explanation of the specific factors that contributed to the selection of the compound, and document the logic behind its recommendations—without revealing the underlying proprietary algorithm [37]. Therefore, using the XAI explanation in combination with the previous patent claim, the company could provide be able to successfully provide a written description of the invention and enable a PHOSITA to make and use the invention.

This hypothetical situation suggests that XAI could reduce the uncertainty posed by the "black box" by providing sufficient transparency into the AI-assisted drug discovery process. It strengthens the legal defensibility of the invention by making the AI's contribution understandable, thereby possibly mitigating the "black box" issue in patent claims involving AI-assisted inventions. Although explainability does not guarantee patentability under Title 35 of the U.S. Code [9], it could assist patent examiners and courts in evaluating the AI's role in the invention and allow inventors to verify that the invention demonstrates a new technological advancement rather than an unexplainable Artificial Intelligence output.

VII Limitations

A. Explainability does not guarantee Patentability

Although XAI has the potential to substantially improve transparency substantially, it does not alter the existing requirements of patent law. AI-assisted inventions must still fulfill the statutory requirements of eligibility, novelty, non-obviousness, and enablement [9]. If a patent holds elements that would otherwise cause it to be unpatentable, XAI cannot prevail [33].

B. Current XAI Methods

Although the field of XAI is rapidly developing, existing techniques are not universally applicable and may therefore provide partial explanations for specific complex ML models [37]. Different explainability methods can yield different interpretations of the same initial model, and some may oversimplify the internal decision-making process [38]. Therefore, explainability should be used as a tool to improve transparency rather than a complete solution to the "black-box" issue. This limitation should be considered when evaluating AI-assisted inventions during patent examination.

VIII Future Implications

As the use of artificial intelligence increases in pharmaceutical drug development, patent law will likely face

growing pressure to address the significant legal implications of AI-assisted inventions [9]. Rather than pursuing comprehensive statutory reform, the USPTO should develop additional guidance on documenting AI-assisted inventions. For instance, USPTO may recognize XAI as sufficient persuasive evidence while examining AI-assisted inventions for patent claims. Pharmaceutical companies may integrate XAI to both improve scientific transparency and to strengthen their legal defense of patent claims involving AI-Assisted inventions. As XAI advances, explainability may become a standard industry practice that enables innovation, patent protection, and transparent decision-making. Future coordination with legal scholars, patent examiners, AI developers, and the pharmaceutical industry will be vital to allow patent law to advance in conjunction with the rapid development of artificial intelligence, whilst maintaining the incentives that drive innovation.

IX Conclusion

The widespread utilization of artificial intelligence into pharmaceutical research poses one of the most significant challenges in modern patent law. As AI increasingly contributes to identifying therapeutic methods, designing drug compounds, and accelerating the overall drug discovery process, the gap between technological developments and existing patent doctrine will widen—unless greater transparency can be achieved.

This article proposes that Explainable Artificial Intelligence (XAI) suggests a practical means of addressing that gap. Rather than explicitly altering the statutory requirements outlined in patent law, XAI poses a potential mechanism for making AI-assisted inventions more understandable and interpretable, without divulging the proprietary value of advanced AI models. If future research, USPTO guidelines, and judicial interpretations align with this suggestion, explainability could become an important tool for strengthening the legal definability of AI-assisted pharmaceutical patents.

Ultimately, the future of AI-assisted drug development will primarily depend on increasing technological developments, and the legal system's ability to preserve the essential exchange underlying the United States patent law system: rewarding innovation with patent protections in exchange for public-disclosure. As artificial intelligence continues to redefine drug discovery, explainability may become the bridge that allows for patent law and innovation to evolve together, rather than apart.

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