Published on 16 July 2025

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND ITS IMPLICATIONS ON PATENTS

[2025] SAL Prac 18

Artificial intelligence ("AI") is transforming the pharmaceutical industry, significantly accelerating drug discovery. This article examines AI's transformative role in early drug discovery and preclinical testing, highlighting its potential to expedite the development of novel therapies. The increasing integration of AI into drug discovery necessitates careful consideration of its implications for the established patent framework. With AI-driven innovation becoming more prevalent, ongoing discussions on contentious issues such as inventorship and patentability are crucial. This article explores these evolving patent considerations, providing a practitioner's perspective on the intersection of AI and intellectual property in the pharmaceutical sector.

Angelina **LIM**[1]
BSc (National University of Singapore), MForSc (University of Western Australia), PhD (Nanyang Technological University);
Senior Patent Examiner, IPOS International Pte Ltd.

I. Introduction

1 The ongoing need for effective treatments drives the search for innovative solutions. Over the past decade, artificial intelligence ("AI") has become an increasingly transformative tool in the pharmaceutical industry. By leveraging machine learning and advanced computational methods, researchers are analysing vast datasets, identifying novel targets and designing promising drug candidates with unprecedented efficiency. AI's influence extends across the entire drug discovery pipeline,

1 The views expressed in this article are the author's personal views only and should not be taken to represent the views of their employer. All errors remain the author's own.

from target identification and validation to predicting molecular interactions and refining drug candidates. Additionally, AI is enhancing clinical trial design by optimising patient selection and predicting outcomes. This comprehensive integration of AI promises to expedite innovation and improve the efficiency of new medicine development.

2 The impact of AI is already being felt. While the discovery and preclinical stages of drug development traditionally take an average of six years, recent analyses suggest AI is significantly compressing this timeline. Boston Consulting Group ("BCG") examined the research pipelines of 20 relatively new AI-intensive pharmaceutical companies between 2010 and 2021.[2] Despite their relative youth, these companies collectively boasted 158 disclosed discovery programs and preclinical assets, compared to the 333 reported by the world's 20 largest pharmaceutical companies. This suggests a dramatic increase in early discovery efficiency and productivity, with these AI-driven companies achieving nearly 50% of the in-house output of industry giants. BCG's analysis, using publicly available data, further noted that multiple AI-based programs completed the discovery and preclinical phase in under four years, significantly outpacing the traditional five-to-six-year average. This demonstrates the immense potential of AI for expediting the development of novel therapies and addressing a range of unmet medical needs.

3 Yet, alongside these advancements, AI's integration into drug discovery presents profound challenges to the established patent system. In the pharmaceutical sector, patent protection is not merely a commercial advantage. It is fundamental to industry survival. Patents, which grant exclusive rights to innovations for 20 years from the filing date, form the cornerstone of the pharmaceutical business model. These rights enable companies to recoup substantial investments in research and development, often spanning over a decade and costing billions of dollars, while also providing incentives for continued innovation. However, traditional patent frameworks, often designed with more

2 Madura K P Jayatunga *et al*, "AI in Small-molecule Drug Discovery: A Coming Wave?" (2022) 21(3) *Nature Reviews Drug Discovery* 175.

conventional drug development processes in mind, may struggle to accommodate the unique nature of AI-driven innovation.

4 The World Intellectual Property Organisation ("WIPO") provides four definitions of AI inventions:[3]

(a) ***AI models or algorithms.*** These relate to core AI technology, forming the foundational instruments that enable AI. Examples include well-known techniques such as machine learning and neural networks.

(b) ***AI-assisted inventions.*** These involve using AI as a tool in the inventive process. The final output of these inventions does not necessarily indicate that an AI tool was used. The output could also have been achieved, albeit with much greater effort, without such a tool. An example would be AlphaFold, a tool used for predicting protein folding.

(c) ***AI-based inventions.*** In these cases, AI is integral to the inventive concept and final output. For example, the da Vinci Surgical System is a robotic surgical platform where AI integration allows for image analysis, surgical planning and real-time adjustments based on the patient's unique anatomy and physiology.

(d) ***AI-generated inventions.*** These refer to inventions made autonomously by AI, with minimal to no human input. A notable example would be the inventions reportedly created by the DABUS system.[4]

5 Complexities surrounding the determination of inventorship and non-obviousness are exacerbated by AI's involvement in AI-assisted and AI-generated inventions. For instance, in AI-generated inventions, when AI significantly contributes to the identification of novel drug targets or the

3 Alexander Cuntz, Carsten Fink & Hansueli Stamm, "Artificial Intelligence and Intellectual Property: An Economic Perspective" (Economic Research Working Paper No 77/2024).

4 DABUS (Device for the Autonomous Bootstrapping of Unified Sentience) is an artificial intelligence system created by Stephen Thaler, who is credited as the inventor in patent applications for two inventions, namely a food container with a fractal profile and a neural flame for attracting attention.

design of new molecules, the question arises: who should be named as the inventor? If AI itself cannot hold inventorship, then who specifically along the drug discovery process should be named as the inventor(s)? The complex interplay between human ingenuity and AI-generated insights is blurring the lines of traditional inventorship.

6 Similarly, the ability of AI to rapidly generate and analyse vast amounts of data raises concerns about the inventiveness of discoveries made with its assistance, *ie*, AI-assisted inventions. In *Nippon Chemiphar Co, Ltd v Shionogi & Co, Ltd*,[5] the Intellectual Property High Court of Japan held that although a general formula was disclosed in the prior art, it encompassed millions of alternatives. The claimed compound was one among 20 million possibilities, and in the absence of a compelling reason to select that specific alternative, the court upheld an inventive step. Following this ruling, discussions emerged about whether the threshold for inventiveness would shift as AI becomes more prevalent in drug discovery.[6] Has that future already arrived?

7 Additionally, an undiscussed yet equally significant issue is the evidentiary support requirement for pharmaceutical patents. With AI-assisted *in silico* modelling becoming increasingly sophisticated, its reliability as a predictive tool continues to improve. This raises a question: will *in silico* data alone be sufficient to establish a drug molecule's claimed therapeutic effects?

8 This article seeks to explore the transformative potential of AI in drug discovery while examining the evolving patent considerations with respect to AI-assisted and AI-generated pharmaceutical inventions.

5 Case No 2016 (Gyo-Ke) 10182, 10184.

6 Ichiro Nakayama, "Patentability and PHOSITA in the AI Era (With a Focus on Inventive Step)", presentation at the 13th IP Conference: Innovation, Intangible Assets During and After the Global Pandemic (30 July 2021) <https://uscipi.org/Events/2021_IP_Seminar/PPT_Collection/07-30_2_Law%20and%20AI/2021-07-30_Ichiro_NAKAYAMA_UploadPPT.pdf> (accessed 16 June 2025).

II. Drug discovery

A. General process

9 The drug discovery and development process is a complex and costly undertaking which can be broadly categorised into four key stages: (a) early drug discovery; (b) preclinical development; (c) clinical development; and (d) regulatory approval. Early drug discovery, the initial and often most challenging phase, encompasses several critical steps. It typically begins with the identification of a disease or unmet medical need, followed by the identification and validation of a relevant biological target, which would be a molecule or process implicated in the disease's pathology. This target validation is crucial, ensuring its suitability for drug intervention. Subsequently, researchers embark on lead compound discovery, commonly screening vast chemical libraries, often using high-throughput methods, to identify molecules that interact with the target. These molecules are then modified to enhance their potency, selectivity and drug-like properties. This iterative optimisation process significantly narrows the field, with only a small fraction of initial candidates, approximately 250 out of 5,000–10,000, progressing to preclinical testing.[7]

10 The preclinical development stage rigorously evaluates the safety and efficacy of lead compounds using *in vitro* (cell culture) and *in vivo* (animal) models. Successful candidates then advance to clinical development, a multi-phase process designed to assess the drug's safety and efficacy in humans. Phase I trials involve a small group of healthy volunteers to determine safety and appropriate dosage. If deemed safe, the drug proceeds to Phase II trials, which evaluate efficacy and further assess safety in a larger group of patients with the target condition. Successful completion of Phase II leads to Phase III trials, involving large patient populations to confirm efficacy, monitor side effects and compare the drug to existing treatments. Positive results from Phase III trials prompt the pharmaceutical company to submit comprehensive preclinical and clinical data to regulatory

7 Biobide, "The Drug Discovery Process: What Is It and Its Major Steps" <https://blog.biobide.com/the-drug-discovery-process> (accessed 16 June 2025).

authorities for review. Regulatory authorities, including the US Food and Drug Administration ("FDA"), the European Medicines Agency ("EMA") and Singapore's Health Sciences Authority ("HSA"), meticulously evaluate the submitted data, often requesting additional information or studies. If the drug is deemed safe and effective, it receives regulatory approval for marketing. Post-market surveillance is subsequently carried out which monitors the drug's safety profile, identifying any rare or long-term adverse effects that may not have been apparent during clinical trials.

11 Some companies or organisations might group these stages slightly differently, but the core activities remain the same. While these stages are presented linearly, there can be overlap and iteration between them. For example, findings from preclinical studies might lead to modifications in the drug discovery phase. As a whole, this intricate process is characterised by a high attrition rate, with only approximately one in 5,000 drug candidates ultimately reaching market approval. The entire process typically spans 12–15 years and requires an investment exceeding $2.5bn, highlighting the significant challenges and resources required to bring a new drug to market.[8]

B. Artificial intelligence in early drug discovery

12 The early drug discovery phase is a pivotal component of pharmaceutical development, comprising of steps such as target identification, lead compound discovery and lead optimisation. This phase is crucial for establishing a strong foundation for subsequent phases of drug development, and the integration of AI is rapidly transforming how researchers approach these tasks.

(1) Target identification

13 The first step in early drug discovery involves identifying relevant biological targets associated with specific diseases.

8 Boston Consulting Group, "Unlocking the Potential of AI in Drug Discovery" (26 June 2023) <https://wellcome.org/reports/unlocking-potential-ai-drug-discovery> (accessed 16 June 2025).

Identifying the correct target is critical, as the success of a drug often depends on its ability to interact effectively with the right biomolecule. AI platforms, such as those developed by Insilico Medicine, harness machine learning algorithms to analyse vast biological datasets which include genomic, transcriptomic, proteomic and metabolomic data. These datasets contain rich information about disease mechanisms, biological pathways and potential therapeutic windows. By uncovering complex patterns and correlations within these datasets, AI can identify novel drug targets that may have been overlooked by conventional methodologies. For example, PandaOmics, a generative biology platform developed by Insilico Medicine, was used to perform a meta-analysis of an endometriosis-associated dataset, searching for new therapeutic targets. Guanylate-binding protein 2, a protein that regulates immune and inflammatory processes, and hematopoietic cell kinase, which is involved in cell proliferation and survival signalling, were revealed for the first time as therapeutic protein targets in endometriosis. Integrin beta 2 was also identified as a potential target for endometriosis, which is also the target of Lifitegrast, an FDA-approved small molecule integrin antagonist currently used in dry eye treatment. This study showcased AI's potential in identifying therapeutic targets and repurposing drug candidates.[9]

(2) Lead compound discovery

14 One way to carry out lead compound discovery is to focus on refining existing compounds or commercially approved drugs using quantitative structure-activity relationships ("QSAR") and screening. Traditional methods of lead compound screening can be time-consuming and resource-intensive, requiring significant investment in resources and time. However, AI technologies, including virtual screening, generative modelling and predictive analytics, are instrumental in streamlining this process.

9 Bonnie Hei Man Liu *et al*, "Utilizing AI for the Identification and Validation of Novel Therapeutic Targets and Repurposed Drugs for Endometriosis" (2025) 12(5) *Advanced Science* (12 December 2024) <https://doi.org/10.1002/advs.202406565> (accessed 1 July 2025).

15 Atomwise exemplifies how AI is transforming lead compound screening through its convolutional neural network model, AtomNet.[10] The model employs virtual high-throughput screening ("vHTS") to rapidly analyse extensive libraries of potential drug molecules, predicting their interactions with target proteins. Traditional high-throughput screening requires that compounds physically exist before testing. However, with the rise of synthesis-on-demand libraries, many commercially available molecules have yet to be synthesised but can be produced and delivered within weeks. These libraries contain trillions of potential compounds, encompassing millions of novel scaffolds that would otherwise remain unexplored in conventional drug discovery. The AI model capitalises on this opportunity by allowing molecules to be tested virtually before synthesis. By using vHTS as the initial screening method, the results inform researchers which molecules are worth synthesising, thus enabling the prioritisation of the most promising compounds for synthesis and testing. This transformative approach significantly expands the chemical space available for drug development, offering a path to discovering novel therapeutics, including those targeting previously "undruggable" proteins.

16 An alternative approach to lead compound discovery would involve generating entirely new molecules, often guided by inverse QSAR and is known as *de novo* drug design. Instead of high-throughput screening, generative AI ("GenAI") models such as Insilico Medicine's Chemistry42 generate entirely new drug-like molecules optimised for specific properties. INS018_055 is a potential anti-fibrotic drug that was discovered and designed using Insilico Medicine's Chemistry42 platform. The novel intracellular target was first identified using PandaOmics and subsequently, Chemistry42 was applied to the target. INS018_055 was the 55th molecule which showed promise and is currently undergoing Phase II clinical trials.[11] Besides Insilico Medicine,

10 Atomwise AIMS Program, "AI is a Viable Alternative to High Throughput Screening: A 318-target Study" (2024) 14(1) *Scientific Reports* <https://doi.org/10.1038/s41598-024-54655-z> (accessed 1 July 2025).

11 Insilico Medicine, "First Generative AI Drug Begins Phase II Trials with Patients" (1 July 2023) <https://insilico.com/blog/first_phase2> (accessed 16 June 2025).

there are a significant number of biopharmaceutical companies, such as Recursion Pharmaceuticals and BioXcel Therapeutics, that employ GenAI in designing new drug molecules. This area of small molecule design is evolving rapidly, with new AI tools and platforms emerging regularly.

(3) Lead optimisation

17 After identifying lead compounds, the optimisation phase focuses on enhancing their pharmacological properties to improve efficacy, selectivity and safety. This stage is critical in ensuring that lead candidates possess the desired characteristics for successful clinical development. AI approaches are increasingly integrated into this process, enabling the prediction of structure–activity relationships ("SARs"), absorption, distribution, metabolism, excretion and toxicity ("ADMET") properties, and off-target effects to streamline optimisation.

18 One of the central challenges in lead optimisation is predicting relative protein–ligand binding affinities, which is vital for structure-based drug design. In May 2024, Google DeepMind and its affiliate, Isomorphic Labs, introduced AlphaFold 3, a revolutionary advancement over its predecessors.[12] Unlike previous versions that focused primarily on protein structure prediction, AlphaFold 3 incorporates a redesigned architecture capable of predicting protein interactions with DNA, RNA and small-molecule ligands. Compared to existing computational tools, it has demonstrated significantly improved accuracy in modelling protein–ligand interactions, protein–nucleic acid binding and antibody–antigen recognition.[13]

19 By integrating advanced AI tools like AlphaFold 3 into lead optimisation, researchers can design more precise and selective drug candidates, accelerating the development of targeted

12 DeepMind, "AlphaFold 3 Predicts the Structure and Interactions of All of Life's Molecules" (8 May 2024) <https://blog.google/technology/ai/google-deepmind-isomorphic-alphafold-3-ai-model/> (accessed 16 June 2025).

13 Josh Abramson *et al*, "Accurate Structure Prediction of Biomolecular Interactions with AlphaFold 3" (2024) 630 *Nature* 493.

therapies and vaccines. These innovations contribute to reducing late-stage clinical failures, ultimately increasing the efficiency of drug discovery and improving the likelihood of successful translation into clinical trials.

(4) First-in-class molecules

20 The transformative impact of AI in early drug discovery is underscored by the emergence of several first-in-class molecules currently undergoing clinical trials. First-in-class drugs introduce novel mechanisms of action, thus offering innovative therapeutic approaches for diseases with high unmet medical needs. AI platforms have significantly accelerated the identification and optimisation of these candidates, reducing development timelines and increasing efficiency.

21 A notable pioneering example would be the earlier discussed INS018_055 by Insilico Medicine, an AI-designed small molecule currently in clinical trials for idiopathic pulmonary fibrosis.[14] A more recent development would be Recursion Pharmaceuticals' REC-1245, a RBM39 degrader developed for the treatment of solid tumours and lymphoma. REC-1245 represents a potential first-in-class therapy, reaching clinical trials within just 18 months, compared to the several years typically required in conventional drug discovery.[15] Notably, in the design process for REC-1245, approximately 200 candidate molecules were synthesised, a drastic reduction compared to the thousands usually required in traditional high-throughput screening.

22 These successes illustrate how AI-driven drug discovery can not only accelerate the identification of first-in-class

14 Feng Ren *et al*, "A Small-molecule TNIK Inhibitor Targets Fibrosis in Preclinical and Clinical Models" (2025) 43 *Nature Biotechnology* 63.

15 Recursion, "Recursion Announces First Patient Dosed in Phase 1/2 Clinical Study of REC-1245, a Potential First-in-class, RBM39 Degrader for Biomarker-Enriched Solid Tumors and Lymphoma" (3 December 2024) <https://www.globenewswire.com/news-release/2024/12/03/2990639/0/en/Recursion-announces-first-patient-dosed-in-Phase-1-2-clinical-study-of-REC-1245-a-potential-first-in-class-RBM39-degrader-for-Biomarker-Enriched-Solid-Tumors-and-Lymphoma.html> (accessed 16 June 2025).

molecules but also streamline their progression into clinical development. By leveraging AI for target identification, lead compound discovery and lead optimisation, pharmaceutical companies are reshaping the landscape of drug discovery, increasing the likelihood of delivering novel and effective therapies at an unprecedented pace.

C. Artificial intelligence in preclinical trials

23 The preclinical stage, a critical bridge between early-stage research and human clinical trials, involves rigorous *in vitro* and *in vivo* testing to assess a drug candidate's ADMET properties. However, this phase is notoriously time-consuming, resource-intensive and prone to inefficiencies, contributing significantly to high drug development attrition rates. AI is increasingly transforming this stage by enhancing predictive modelling, improving experimental efficiency and optimising decision-making processes.

24 Traditionally, AI applications in toxicology have been dominated by data processing for pattern identification and prediction, exemplified by QSARs. While valuable, these models often provide limited single-endpoint predictions, contrasting with the multifaceted toxicological insights derived from animal-based assessments. However, novel AI-driven approaches are addressing this limitation. AnimalGAN, developed by the FDA, generates synthetic animal data by training on extensive datasets from 6,442 rats across 1,317 treatment scenarios. This enables "virtual experiments" and large-scale simulations, offering insights beyond traditional methods. In a comparative study using 38 clinical pathology measurements, AnimalGAN demonstrated significantly lower mean square error compared to individual QSAR models, showcasing its ability to provide comprehensive, multi-endpoint predictions.[16] Furthermore, in alignment with regulatory guidelines requiring rodent and

16 Xi Chen *et al*, "A Generative Adversarial Network Model Alternative to Animal Studies for Clinical Pathology Assessment" (2023) 14(1) *Nature Communications* (6 November 2023) <https://doi.org/10.1038/s41467-023-42933-9> (accessed 1 July 2025).

non-rodent species for toxicology studies,[17] the Virtual Second Species project is seeking to develop an AI-powered virtual dog, trained on historical dog test data, complementing AnimalGAN's rodent-focused approach.[18]

25 Despite these advancements in refining animal-based predictions, the inherent limitations of animal models in predicting human outcomes remain a critical concern. A concept known as Trans-Species Modeling Theory highlights the unpredictability of extrapolating animal data to humans.[19] This is illustrated by the historical case of aspirin, which exhibited toxicity in rodents and canines but is safe and effective in humans.[20] To address this fundamental challenge, the Virtual Human Platform for Safety Assessment project is developing a virtual human platform[21] ("VHP"), leveraging human-specific data to evaluate chemical and pharmaceutical safety. By integrating diverse datasets – including human physiology, clinical and epidemiological findings, *in vitro* and *in silico* model outputs, chemical properties and biological pathway perturbations – the VHP aims to transition from animal-centric to human-centric safety assessments. This platform uses AI to process and synthesise complex datasets, generating predictive outputs based on disease state, life course exposure and demographics. The continuous expansion of biomedical knowledge and advancements in New Approach Methodologies ("NAMs") are driving the development of these

17 Rostam Namdari *et al*, "Species Selection for Nonclinical Safety Assessment of Drug Candidates: Examples of Current Industry Practice" (2021) 126 *Regulatory Toxicology and Pharmacology* (27 August 2021) <https://doi.org/10.1016/j.yrtph.2021.10502> (accessed 1 July 2025).

18 National Centre for the Replacement, Refinement & Reduction of Animals in Research, "£1.6M Awarded to Develop a Virtual Second Species" (13 March 2023) <https://nc3rs.org.uk/news/ps16m-awarded-develop-virtual-second-species> (accessed 16 June 2025).

19 Ray Greek & Lisa A Kramer, "The Scientific Problems with Using Non-human Animals to Predict Human Response to Drugs and Disease" in *Animal Experimentation: Working Towards a Paradigm Change* (Kathrin Herrmann & Kimberley Jayne eds) (Brill, 2019) ch 17 at pp 391–416.

20 Rebecca Ram, "Extrapolation of Animal Research Data to Humans: An Analysis of the Evidence" in *Animal Experimentation: Working Towards a Paradigm Change* (Kathrin Herrmann & Kimberley Jayne eds) (Brill, 2019) ch 15 at pp 341–375.

21 Anne Kienhuis *et al*, "The Virtual Human Platform for Safety Assessment (VHP4Safety) Project: Next Generation Chemical Safety Assessment Based on Human Data" (2025) 42(1) ALTEX 111.

human biology-based approaches. Ultimately, the VHP holds the potential to reform preclinical trials, diminishing reliance on animal testing and enhancing the accuracy of human safety predictions for novel pharmaceuticals.

III. Implications on patents

A. Inventorship

26 When submitting a patent application, it is a fundamental requirement to identify the inventor(s) of the invention. In Singapore, failure to comply could result in the application being deemed abandoned.[22] If an error in naming the inventors occurred in good faith, a correction may be submitted. However, intentional misrepresentation of inventorship can compromise the enforceability of a patent.[23] While jurisdictions may differ in their specific terminology and testing methods for determining inventorship, the underlying goal remains consistent: to identify the individual(s) who contributed to the invention's conception. To be recognised as an inventor, one must have contributed to the formation of the inventive idea itself.

27 The increasing integration of AI in drug discovery raises complex questions regarding inventorship. A key consideration is the extent of AI's contribution to the inventive concept. In AI-assisted inventions, AI functions as an advanced analytical tool, aiding pattern recognition, hypothesis generation and automation. The human researchers direct and interpret the AI-generated outputs, ensuring that inventive input originates from a natural person. In such cases, patentability is clear: the human scientist is the rightful inventor, and AI is merely a highly capable but uninventive assistant.

28 However, for AI-generated inventions, this distinction between human and AI contributions to innovation is becoming increasingly blurred. AI is now more than just a tool simply for

22 Patents Act 1994 (2020 Rev Ed) s 24(2).
23 *Frank's Casing Crew & Rental Tools, Inc v PMR Technologies, Ltd* 292 F 3d 1363 (Fed Cir, 2002).

automation and data analysis. AI-designed drug molecules, particularly those identified through deep learning and generative models, often exhibit structural novelty, unique binding affinities and pharmacological properties that were neither explicitly programmed nor easily conceived by human scientists. Examples include the first-in-class molecules by companies like Insilico Medicine and Recursion Pharmaceuticals, where AI not only suggests viable drug candidates but also designs new chemical scaffolds that are absent in existing chemical libraries.[24] In these cases, the AI system's contribution extends beyond computational efficiency. It is able to actively generate innovative and non-obvious solutions, contributing to the conception of the invention. Much like how ChatGPT-4 overcame the Turing test,[25] GenAI appears to be encroaching on the once-exclusive domain of human ingenuity.

29 This issue on inventorship was brought to global attention through the DABUS case, where AI was listed as the inventor on patent applications filed in multiple jurisdictions. Section 2(1) of the Singapore Patents Act 1994[26] defines an "inventor" as "the actual deviser of the invention" and the courts have interpreted this to mean "the *natural person* who came up with the inventive concept"[27] [emphasis in original]. Courts and patent offices worldwide, including the US, UK and European Union, rejected the applications on the basis that only humans qualify as inventors under existing patent laws.[28] The underlying policy rationale is that patent systems are designed to incentivise human creativity and innovation by granting exclusive rights to inventors. AI, lacking legal personhood and an ability to exercise ownership, cannot fulfil the requirements for inventorship.

24 Olga Kapustina *et al*, "User-friendly and Industry-integrated AI for Medicinal Chemists and Pharmaceuticals" (2024) 2 *Artificial Intelligence Chemistry* 1.

25 Qiaozhu Mei *et al*, "A Turing Test of Whether AI Chatbots are Behaviorally Similar to Humans" (2024) 121(9) *Proceedings of the National Academy of Sciences* (22 February 2024) <https://doi.org/10.1073/pnas.2313925121> (accessed 1 July 2025).

26 2020 Rev Ed.

27 *Energenics Pte Ltd v Musse Singapore Pte Ltd* [2013] SGHCR 21 at [24].

28 WIPO Standing Committee on the Law of Patents, "Artificial Intelligence (AI) and Inventorship" (13 September 2023).

30 This raises a crucial question: if an AI system makes a non-obvious inventive leap that human researchers may not have considered, should it be credited as an inventor, or is it still just a tool? Some argue that even in cases where AI has generated an entirely novel solution, it remains an instrument, albeit an exceptionally powerful one, deployed by human researchers in pursuit of discovery.[29] Others contend that denying AI inventorship in cases of true AI-generated discovery may discourage innovation by failing to appropriately recognise AI's contribution to scientific advancement.[30]

31 Rather than viewing AI as a standalone inventor, a more pragmatic legal approach might be to classify AI as an advanced tool that augments human creativity, much like computational chemistry software, X-ray crystallography, or deep neural networks for structural biology. Although AI platforms can design molecules beyond human intuition, their operation is still fundamentally guided, refined and interpreted by human scientists. The role of human expertise in directing AI systems, validating outputs and making final drug development decisions suggests that AI, no matter how creative, remains a means to an end rather than an independent innovator. Even then, critical questions regarding the attribution of inventorship persist. Would the scientist training the AI model, the one deciding the prompts or the one selecting the most appropriate AI-designed drug molecule be considered as inventor(s)?[31] As GenAI continues to push the boundaries of pharmaceutical innovation, the question of who (or what) qualifies as an inventor will remain a pivotal issue in shaping the future of patent law and scientific research.

29 Tan Tee Jim SC, "Artificial Intelligence as Inventor?" (2024) 36 SAcLJ 346.

30 Juan Gorraiz, "Acknowledging the New Invisible Colleague: Addressing the Recognition of Open AI Contributions in Scientific Publishing" (2025) 19(2) *Journal of Informetrics* (3 February 2025) <https://doi.org/10.1016/j.joi.2025.101642> (accessed 1 July 2025); Ryan Abbott, "I Think, Therefore I Invent: Creative Computers and the Future of Patent Law" (2016) 57(4) *Boston College Law Review* 1079.

31 Jordan Phelan & Jon Cousin, "The Challenge of AI Inventorship in Healthcare" <https://www.drugdiscoverytrends.com/the-challenge-of-ai-inventorship-in-healthcare/> (accessed 16 June 2025).

B. Non-obviousness

32 Intertwined with inventorship is the assessment of inventive step. The presence of an inventive step or non-obviousness of an invention is one of the many statutory requirements for a patent grant. Unlike novelty, which comparatively is a more straightforward assessment of whether something existed before, non-obviousness is a frequently litigated aspect of patent law. Although legal frameworks such as the Windsurfing or Pozzoli tests and the problem-solution approach provide guidance, there remains interpretative leeway. As noted by V K Rajah JA in *First Currency Choice*:[32]

> … Quite often, it is difficult, in practice, to break down the Windsurfing test ([41] above) into its component parts. Thus, while the Windsurfing test remains a useful guide, it is no more than that. Above all, it should be borne in mind that the Windsurfing test is merely a manifestation of judicial inventiveness on how best to pragmatically interpret and elucidate the requirements of s 15 of the Act.

33 An invention is generally deemed to involve an inventive step if it is not obvious to a person skilled in the art ("PSA"). The definition of the PSA is thereby crucial in determining obviousness, and as a result, this legal construct has been extensively analysed in case law. Key issues regarding the PSA include the level of expertise required, the extent of general knowledge attributed to them, and whether they can represent a team rather than an individual. As technology evolves, so too do the tools available to the PSA. It has been suggested that with the increasing adoption of AI systems, the PSA may reasonably be expected to use AI, regardless of whether applicants actually employed such technology in developing the invention.[33] The question then arises: should AI systems, including GenAI, be

32 *First Currency Choice Pte Ltd v Main-Line Corporate Holdings Ltd* [2008] 1 SLR(R) 335 at [45].

33 Ichiro Nakayama, "Patentability and PHOSITA in the AI Era (With a Focus on Inventive Step)", presentation at the 13th IP Conference: Innovation, Intangible Assets During and After the Global Pandemic (30 July 2021) <https://uscipi.org/Events/2021_IP_Seminar/PPT_Collection/07-30_2_Law%20and%20AI/2021-07-30_Ichiro_NAKAYAMA_UploadPPT.pdf> (accessed 16 June 2025).

considered standard tools of the trade for a skilled person in drug discovery? If so, would the threshold for inventiveness be raised, given that AI can rapidly generate and optimise molecular structures? Also, if GenAI is not yet regarded as a standard tool, how prevalent must its use become before it is deemed an ordinary part of the PSA's toolkit? These considerations could significantly impact the assessment of inventive step. As the PSA's toolkit rapidly evolves, patent examiners face an increasing challenge in appropriately evaluating inventiveness.

34 Acknowledging the emerging complexities surrounding AI and intellectual property ("IP"), the UK Government launched a public consultation in 2021.[34] Notably, most respondents agreed the PSA should be considered to have access to a range of tools, including AI technologies. Moreover, it was commented that as AI tools improve, the standard of obviousness may shift, with more modifications being deemed obvious. In 2024, the US Patent and Trademark Office similarly sought public input on how AI proliferation affects prior art and the concept of a person having ordinary skill in the art.[35] As more jurisdictions worldwide engage in concurrent discussions, the challenge remains to develop a consistent and balanced approach that acknowledges AI's transformative capabilities while maintaining a robust and fair patent framework.

C. In silico *data as evidentiary support*

35 When filing for patent protection for drug molecules, there needs to be evidence to prove that these molecules are indeed doing as they claim. To fulfil this requirement, applicants

34 Intellectual Property Office, "Consultation Outcome: Government Response to Call for Views on Artificial Intelligence and Intellectual Property" (23 March 2021) <https://www.gov.uk/government/consultations/artificial-intelligence-and-intellectual-property-call-for-views/government-response-to-call-for-views-on-artificial-intelligence-and-intellectual-property#conditions-for-grant-of-a-patent> (accessed 16 June 2025).

35 United States Patent and Trademark Office, "Impact of the Proliferation of AI on Prior Art and Person Having Ordinary Skill in the Art (PHOSITA) Listening Session" <https://www.uspto.gov/sites/default/files/documents/impact-of-the-proliferation-of-ai-on-prior-art-listening-session-slides.pdf> (accessed 16 June 2025).

typically include efficacy data in the specification, demonstrating the binding of such drug molecules to their target sites and the subsequent effects that lead to the claimed therapeutic outcome. In Singapore, pharmaceutical patent applications commonly employ first or second medical use claims, which, according to the Examination Guidelines for patent applications at the Intellectual Property Office of Singapore ("IPOS"), must be supported by adequate evidence of likely efficacy as filed.[36]

36 The advent of highly accurate *in silico* prediction tools, such as AlphaFold 3, raises the question of whether such computational evidence alone would suffice for demonstrating efficacy. Patents are typically filed during the preclinical stage, involving animal models, or in the early phases of Phase II clinical trials, following initial human efficacy testing. Given the increasing reliability of *in silico* predictions, researchers may be inclined to file patent applications earlier, potentially prior to conducting extensive preclinical trials. IPOS's Examination Guidelines for patent applications acknowledge that *in silico* modelling data may be considered a credible form of efficacy support for medical uses. However, the sufficiency of such evidence is determined on a case-by-case basis, taking into account the prevailing state of the art.[37] While there is no local case law on this specific issue, decisions from the European Patent Office could provide some insights. The Board of Appeal in T 801/06 affirmed that a "claimed therapeutic effect may be proven by any kind of data as long as they clearly and unambiguously reflect the therapeutic effect".[38] Similarly, T 1642/06 emphasised the principle of free evaluation of evidence, stating that clinical demonstration of a therapeutic effect is not a prerequisite.[39] Rather, the determinative factor is

36 Intellectual Property Office of Singapore, "Examination Guidelines for Patent Applications at IPOS" (October 2023) at paras 8.132 and 8.179.

37 Intellectual Property Office of Singapore, "Examination Guidelines for Patent Applications at IPOS" (October 2023) at para 8.135.

38 Cancer treatment with HSV mutant/CRUSADE 04-03-2009 Case T 0801/06/2009, ECLI:EP:BA:2009:T080106.20090304 at [28] <https://www.epo.org/boards-of-appeal/decisions/pdf/t060801eu1.pdf> (accessed 19 June 2025), European Patent Office, Boards of Appeal.

39 Sigma receptor/SPRUCE BARBARA, *et al* 23-08-2007 Case T 1642/06/2007, ECLI:EP:BA:2007:T164206.20070823 at [2.2] <https://www.epo.org/boards-of-appeal/decisions/pdf/t061642eu1.pdf> (accessed 19 June 2025), European Patent Office, Boards of Appeal.

whether the skilled person, based on generally accepted models, can directly and unambiguously infer the claimed therapeutic application from the data provided, such as pharmacological, pharmaceutical, *in vitro* or animal model data.

37 Wet-lab data is generally perceived as more robust than *in silico* data due to the latter's reliance on predictive modelling. Consequently, applicants often supplement *in silico* findings with *in vitro* and/or *in vivo* data to bolster their evidentiary support. However, this perception could have changed with the demonstrated reliability of *in silico* prediction tools. Xu Jinbo, Professor at the Toyota Technological Institute at Chicago who advanced convolutional networks, noted: "Biologists now believe our prediction results. Before, biologists always suspected if our prediction is reliable."[40] In this increasingly competitive pharmaceutical landscape coupled with the heightened credibility of AI-assisted tools like AlphaFold 3, applicants may be emboldened to rely solely on *in silico* data. While patent offices may be satisfied with such evidence during examination of the patent applications, this could potentially lead to increased challenges from third parties regarding the sufficiency of such evidence, raising concerns about its evidentiary weight. It remains an open question whether the continuous improvement in AI accuracy will eventually resolve these concerns or give rise to a new evidentiary standard that requires legal consideration.

IV. Conclusion

38 The integration of AI into drug discovery is reshaping pharmaceutical research and development, improving efficiency and offering new approaches to longstanding medical challenges. This technological revolution compels those involved in patents to critically examine the implications of these advancements. While the issues of inventorship, non-obviousness and evidentiary support each warrant in-depth discussion, the present analysis

40 Yasemin Saplakoglu, "How AI Revolutionized Protein Science, but Didn't End It", *Quanta Magazine* (26 June 2024) <https://www.quantamagazine.org/how-ai-revolutionized-protein-science-but-didnt-end-it-20240626/> (accessed 16 June 2025).

provides a brief exploration of these complex topics in the context of AI-assisted and AI-generated pharmaceutical inventions. Challenges surrounding inventorship and non-obviousness have sparked extensive debate. Yet, many questions remain unanswered and greater clarity is needed.

39 With the field of AI experiencing exponential growth, the definitions of AI provided by WIPO will likely expand beyond the current four. The relentless advancement of AI technology will undoubtedly continue to test the boundaries of IP, raising even more pressing questions for patents, including inventorship. It is therefore imperative to not only continue this discourse to seek answers, but to also deepen the conversation to ensure that the patent framework remains fit for purpose, effectively balancing the encouragement of genuine innovation with the preservation of established legal principles.