

The Use of Artificial Intelligence in Drug Discovery: Patent Strategy Considerations and Policy Approaches to Improve Legal Certainty

Fè Laura*, Norga Alice

I. Introduction

Artificial intelligence (AI) is no longer a peripheral tool in pharmaceutical research. It is increasingly embedded in the way new therapeutic opportunities are identified, evaluated and advanced. AI systems are used to analyze biological data, identify disease targets, predict protein interactions, design candidate molecules, optimize lead compounds and support decisions about which candidates should proceed to experimental testing.¹ In a sector where innovation is expensive, uncertain and slow, these tools promise a significant acceleration of the research and development process.^{2,3}

The practical uptake of AI in drug development is no longer merely prospective. The FDA reports receiving more than 500 submissions for drugs and biological products with AI components between 2016 and 2023, spanning the product lifecycle.⁴ Patent data points the same way. The EPO reports that AI-related filings grew by 9.5% in 2025, and that annual

* Executive Director, Murgitroyd, Munich, Germany

¹ Alexandre Blanco-González et al., "The Role of AI in Drug Discovery: Challenges, Opportunities, and Strategies," *Pharmaceuticals* 16, no. 6 (2023): 891, <https://doi.org/10.3390/ph16060891>

² Tian Xie et al., "Artificial Intelligence in Drug Development: From Molecular Discovery to Precision Medicine." *Genes & Diseases*, 102402, <http://doi.org/10.1016/j.gendis.2026.102402>

³ R.S.K. Vijayan et al., "Enhancing Preclinical Drug Discovery with Artificial Intelligence." *Drug Discovery Today* 27 (4). <https://doi.org/10.1016/j.drudis.2021.11.023>

⁴ "FDA Proposes Framework to Advance Credibility of AI Models Used for Drug and Biological Product Submissions," US Food and Drug Administration, published January 6, 2025, <https://www.fda.gov/news-events/press-announcements/fda-proposes-framework-advance-credibility-ai-models-used-drug-and-biological-product-submissions>.

volumes are now 24 times those of a decade ago.⁵ Neither the EPO nor the USPTO publishes an official series isolating AI-related biopharma applications and grants, so these figures should be read as indicators of the wider technological and patenting context rather than as counts of AI-drug patents.

This technological shift has direct consequences for patent law. Pharmaceutical innovation depends on strong, predictable patent protection to offset long development timelines, high failure rates, easy reverse engineering, and substantial financial investment, making the industry uniquely reliant on enforceable exclusivity. Patent rights help convert early-stage scientific insight into assets capable of attracting funding, supporting collaboration and enabling market entry. If the legal framework becomes uncertain when AI contributes materially to the inventive process, the commercial incentives that underpin life-sciences innovation may be weakened resulting in capital flowing out of entire industries.⁶

The European patent system, principally governed by the European Patent Convention (EPC), does not exclude inventions developed with AI assistance. It nevertheless remains built around human-centered concepts. Under current EPO practice, an inventor must be a natural person. Sufficiency of disclosure under Article 83 EPC is assessed by whether the skilled person can carry out the invention across its claimed scope without undue burden. Inventive step under Article 56 EPC is evaluated from the perspective of the notional skilled person or team, whose ordinary tools and common general knowledge may evolve as AI becomes routine in a particular technical field. Although these concepts are adaptable, they were not designed for workflows in which AI systems can generate, rank, or optimize technical solutions at scale.

The tension is particularly visible in AI-assisted drug discovery. Research teams may define the biological problem, select or curate training data, choose model architecture, set constraints,

⁵ “Insight into Computer Technologies,” EPO Technology Dashboard 2025, European Patent Office, accessed October 11, 2026, <https://www.epo.org/en/about-us/statistics/technology-dashboard-2025/insight-computer-technologies>.

⁶ Mark F. Schultz, “Declining Patent Reliability and Venture Capital Reallocation,” in *Bringing Medicines to Life: How Intellectual Property Enables Innovation in the Life Sciences*, ed. Jonathan M. Barnett and Bowman Heiden (Cambridge: Cambridge University Press, forthcoming).

interpret outputs and validate promising compounds. At the same time, the AI system may produce the molecular structure, propose a synthetic route or identify an unexpected technical relationship. In such cases, the legal concern is not whether AI was used, but whether the human contribution can be characterized, evidenced and claimed in a way that satisfies established patent law requirements.

These developments also expose a policy trade-off that recurs throughout this article. Patent law should remain capable of rewarding genuine human technical contribution and supporting the investment, licensing and collaboration needed to turn an AI-assisted discovery into an approved medicine. At the same time, if familiar doctrines are applied too generously to large-scale computational generation, patents may confer broad exclusivity over outputs that were routine to generate or insufficiently disclosed; if they are applied too restrictively, firms may shift valuable data, models and discovery know-how into trade secrecy or contractual control.

Recent guidance and policy initiatives show that patent offices and international organizations are beginning to address these questions. For example, the EPO Guidelines have clarified that AI and machine-learning, in spite of being abstract mathematical or computational models, can be patentable where their use contributes to a technical solution to a technical problem.⁷ The USPTO's revised guidance confirms that the same inventorship standard applies irrespective of whether AI was used and that only natural persons may be inventors.⁸ AIPPI Resolution Q272 suggests that to foster innovation, inventions made using AI should not be excluded from patent protection, even if there is no sufficient human contribution to name an inventor, provided a "natural or legal person" is named as the applicant.⁹ AIPPI Resolution

⁷ European Patent Office. "Guidelines for Examination in the European Patent Office: Artificial Intelligence and Machine Learning.", European Patent Office, accessed 14 October 2026, https://www.epo.org/en/legal/guidelines-epc/2026/g_ii_3_3_1.html

⁸ United States Patent and Trademark Office, *Revised Inventorship Guidance for AI-Assisted Innovation* (Washington, DC: U.S. Department of Commerce, 2025), <https://public-inspection.federalregister.gov/2025-21457.pdf>.

⁹ AIPPI, Resolution Q272, "Inventorship of inventions made using Artificial Intelligence" (2020), <https://www.aippicanada.org/wp-content/uploads/2020/12/Adopted-Resolution-Q272-Patents-Inventorship-of-inventions-made-using-Artificial-Intelligence.pdf>.

Q276 proposes that AI inventions should generally be assessed under ordinary patent-law principles, not under a special or stricter AI-specific regime.¹⁰

Against this background, this article examines whether European patent law concepts can adequately support AI-assisted pharmaceutical innovation. It focuses on three main challenges: identifying a natural person whose contribution supports inventorship; enabling the skilled person to reproduce the claimed technical effect without undue burden, despite the data dependence of many AI systems; and assessing inventive step when AI tools may form part of the ordinary capabilities of the skilled person. It further considers how AI use should be disclosed in patent applications in connection with drug-discovery inventions, particularly where regulatory transparency and patent strategy may point in different directions.

The article's aim is both practical and policy-oriented: to identify the issues patent applicants face and the disclosure choices they should make, and to consider how patent offices and policymakers could improve predictability without departing from established patent-law principles. Although the focus of this article is on the European patent system under the EPC, international examples are used as points of comparison because pharmaceutical inventions are commonly filed across multiple jurisdictions, and differences in patent office approaches can shape in-house filing strategy, documentation, and decision-making.

II. AI-Assisted Drug Discovery and the Patent-Strategy Problem

Drug discovery has always involved the management of uncertainty. Researchers must identify a biologically relevant target, understand its role in disease, discover or design molecules capable of modulating that target, optimize those molecules for potency and selectivity, and assess properties such as toxicity, stability, bioavailability and manufacturability. Each stage involves large volumes of data, complex biological relationships and a high risk that promising early results will not translate into safe and effective medicines.

AI may support almost every stage of the drug-discovery pipeline. In target identification, machine-learning systems can analyze genomic, proteomic, clinical and phenotypic datasets to

¹⁰ AIPPI, Resolution Q276, “Inventiveness and Sufficiency of Disclosure in AI Inventions”, October 22, 2021, <https://www.aippi.org/content/uploads/2021/11/SQ-276-Resolution.pdf>.

detect disease-associated patterns or prioritize biological pathways.¹¹ In hit discovery and virtual screening, AI can search large chemical spaces and predict which molecules are likely to bind to a target. In lead optimization, generative models can propose new structures with improved potency, selectivity or pharmacokinetic properties.¹² Other systems may predict toxicity, metabolic stability, synthetic accessibility or likely off-target effects.¹³ More advanced platforms integrate several of these functions into iterative design–make–test–learn cycles.¹⁴ For the purposes of this article, “AI-assisted drug discovery” is used broadly to cover all the above steps. “AI-generated output” refers to a model-generated candidate, ranking, prediction, hypothesis or design proposal.

These applications do not remove the need for human scientific judgment. AI-generated outputs must still be evaluated against biological plausibility, chemical feasibility, regulatory expectations and commercial strategy. A candidate molecule suggested by an AI system is not automatically a viable drug candidate. Researchers must decide which outputs to trust, which compounds to synthesize, which assays to perform and how to interpret experimental results.

Market examples illustrate the diversity of AI-assisted drug-discovery models. Insilico Medicine, an AI-driven biotech company, is often cited as an end-to-end example: its Pharma.AI platform combines target identification, molecular generational and clinical-trial prediction,¹⁵ and its fibrosis candidate Rentosertib has been presented as a prominent case in which both the target and the molecule were identified through an AI-assisted workflow.¹⁶ Recursion Pharmaceuticals, an oncology biotech company, applies high-throughput phenotypic screening and machine learning to map relationships between cellular perturbations

¹¹ Vivek Kaul, Sarah Enslin, and Seth A. Gross, "History of Artificial Intelligence in Medicine," *Gastrointestinal Endoscopy* 92, no. 4 (October 2020): 807–812, <https://doi.org/10.1016/j.gie.2020.06.040>.

¹² Kaul, Enslin and Gross, “History of Artificial Intelligence”

¹³ Kaul, Enslin and Gross, “History of Artificial Intelligence”

¹⁴ Kaul, Enslin and Gross, “History of Artificial Intelligence”

¹⁵ "Pharma.AI Suite," Insilico Medicine, accessed August 4, 2026, <https://pharma.ai/>.

¹⁶ "Rentosertib: Treating Fibrotic Diseases," Insilico Medicine, accessed August 4, 2026, <https://insilico.com/interactive/drugs/rentosertib>.

and disease biology;¹⁷ its acquisition of Exscientia, an automated drug-design and precision-medicine company, brought phenomics, automation and AI-designed chemistry together.¹⁸ Schrödinger represents a different model: as a computational platform company, it combines physics-based molecular simulation with machine-learning tools, and it operates a software-plus-pipeline business model used by pharmaceutical partner.¹⁹ Other notable examples include the AI company Isomorphic Labs, which builds on the protein-structure prediction and generative design capabilities associated with AlphaFold;²⁰ the therapeutics company Generate:Biomedicines, which focuses on protein and antibody design;²¹ the pharma company Atomwise, known for AI-enabled virtual screening;²² and BenevolentAI, an AI-enabled drug discovery company, which has used knowledge graphs and machine learning for target identification and drug-repurposing hypotheses.²³

These specialist providers do not operate in isolation. Large pharmaceutical companies increasingly rely on collaborations with them, combining proprietary biological, chemical, and clinical datasets with external computational tools: Sanofi has partnered with both Exscientia

¹⁷ "Decoding Biology Demands a Bold Approach," Recursion, accessed August 4, 2026, <https://www.recursion.com/mission>.

¹⁸ "Recursion and Exscientia Enter Definitive Agreement to Create a Global Technology-Enabled Drug Discovery Leader with End-to-End Capabilities," Recursion, accessed August 4, 2026, <https://ir.recursion.com/news-releases/news-release-details/recursion-and-exscientia-enter-definitive-agreement-create>.

¹⁹ "The Leading Computational Platform for Molecular Discovery and Design," Schrödinger, accessed August 4, 2026, <https://www.schrodinger.com/platform/>.

²⁰ "Solve All Disease," Isomorphic Labs, accessed August 4, 2026, <https://www.isomorphiclabs.com/>.

²¹ "Pushing Boundaries in Everything That We Do," Generate:Biomedicines, accessed August 28, 2026. <https://generatebiomedicines.com/about-us/>.

²² "The Art of Drug Hunting, Powered by ML," Atomwise, accessed August 28, 2026. <http://www.atomwise.com>.

²³ "Life Science Intelligence," BenevolentAI, accessed August 4, 2026, <https://www.benevolent.com/>.

and Atomwise for AI-enabled small-molecule discovery,²⁴ Bayer with Recursion,²⁵ Eli Lilly and Novartis separately with Isomorphic Labs,²⁶ and AstraZeneca with BenevolentAI for target identification and knowledge-graph-based discovery.²⁷

In October 2025, Eli Lilly announced an NVIDIA-based “AI factory”, intended to support the training and deployment of models across drug discovery and development.²⁸ Selected models are made available through Lilly TuneLab, a platform offering participating companies access to models trained on decades of Lilly research data, including preclinical pharmacokinetic and toxicology data. Participants can contribute training data through privacy-preserving federated learning, so that the shared models may improve without Lilly or other participants directly accessing their proprietary molecular information.²⁹ This model suggests

²⁴ "Exscientia and Sanofi Establish Strategic Research Collaboration to Develop AI-Driven Pipeline of Precision-Engineered Medicines," *Sanofi*, January 7, 2022, <https://www.sanofi.com/en/media-room/press-releases/2022/2022-01-07-06-00-00-2362917>.

²⁵ "Bayer Collaborates with Recursion to Strengthen Digital Drug Discovery and Advance New Therapies for Fibrotic Diseases," *Bayer*, September 9, 2020, <https://www.bayer.com/media/en-us/bayer-collaborates-with-recursion-to-strengthen-digital-drug-discovery-and-advance-new-therapies-for-fibrotic-diseases/>.

²⁶ "Isomorphic Labs Kicks Off 2024 with Two Pharmaceutical Collaborations," *Isomorphic Labs*, January 7, 2024, <https://www.isomorphiclabs.com/articles/isomorphic-labs-kicks-off-2024-with-two-pharmaceutical-collaborations>.

²⁷ "AstraZeneca Starts Artificial Intelligence Collaboration to Accelerate Drug Discovery," *AstraZeneca*, April 30, 2019, <https://www.astrazeneca.com/media-centre/press-releases/2019/astrazeneca-starts-artificial-intelligence-collaboration-to-accelerate-drug-discovery-30042019.html>.

²⁸ "Lilly Partners with NVIDIA to Build the Industry's Most Powerful AI Supercomputer, Supercharging Medicine Discovery and Delivery for Patients," *Eli Lilly and Company*, October 28, 2025, <https://investor.lilly.com/news-releases/news-release-details/lilly-partners-nvidia-build-industrys-most-powerful-ai>.

²⁹ "Lilly Launches TuneLab Platform to Give Biotechnology Companies Access to AI-Enabled Drug Discovery Models Built through over \$1 Billion in Research Investment," *Eli Lilly and Company*, September 9, 2025, <https://investor.lilly.com/news-releases/news-release-details/lilly-launches-tunelab-platform-give-biotechnology-companies>.

that a competitive advantage may arise not only from a patented molecule or algorithm, but also in the scale and quality of proprietary datasets, the infrastructure used to train models, and control over the platform through which models are accessed.

AI-assisted drug discovery may therefore give rise to three distinct types of claimed invention: a drug or therapeutic use discovered with AI, an AI-based screening or optimization method, or the underlying AI model, architecture or training method. Each raises different issues: human inventorship and therapeutic support for the first; disclosure and inventive step for the second; and patent eligibility, technical character and possible trade-secret protection for the third. The analysis therefore depends not merely on whether AI was used, but on what the applicant seeks to protect.

Disclosure can both strengthen and weaken a patent application. Explaining AI's role may support inventorship, reproducibility and the technical contribution, while unnecessary detail may expose proprietary assets or suggest that the result followed from routine computational methods.

Effective protection therefore often combines patents with trade secrets. Confidential treatment may be particularly important for training data, prompts, fine-tuning and validation workflows, as well as molecular structures, target profiles, assay results and negative findings that reveal a research program's direction before filing. This balance should be assessed before filing. Applicants should disclose what is needed to support inventorship, sufficiency and inventive step, while preserving non-essential training data, model-development choices and negative results as confidential know-how where possible.

A related pre-filing risk arises when unpublished technical information is submitted to an external AI tool. Public services may retain prompts, allow provider or human access, use content for training, or impose no duty of confidentiality. If an enabling disclosure thereby becomes available to a person free to use or disseminate it before the filing or priority date, novelty may be at risk. The assessment depends on the service terms, account settings, access arrangements, subsequent use and available evidence.

*Trinidad v. OpenAI, Inc.*³⁰ highlights a related trade-secret risk. The Northern District of California dismissed the claim because the alleged proprietary frameworks had been shared through a public AI tool that imposed no duty of confidentiality. The court found that this was inconsistent with taking reasonable steps to keep the information secret. The decision does not mean that every AI prompt becomes patent prior art. It does, however, support filing before sharing enabling information and using only approved enterprise or internal systems with clear safeguards on confidentiality, access, retention and model training. Organizations should also adopt AI-use policies and keep records of the tool, account, settings, terms and information submitted.

Contracts are central to this strategy for collaborative AI-assisted drug discovery.³¹ Agreements with platform providers, academic partners, cloud providers and pharmaceutical collaborators should address ownership and permitted use of training data, derived data, annotations, model outputs, fine-tuned models and validation results. For example, where a pharmaceutical company provides proprietary assay data to an external AI-platform provider to train or fine-tune a model that proposes candidate molecules, the collaboration agreement should specify whether the provider may reuse the assay data or derived embeddings for other customers, who owns the fine-tuned model and generated candidates, and which party may use validation results in patent filings or subsequent research.

III. Inventorship: Identifying and Preserving the Human Contribution

A. The legal standard

Inventorship is the most obvious area in which AI-assisted drug discovery tests the limits of the European patent system, which has traditionally treated invention as an act of human intellectual creation. Although the European Patent Convention does not establish a substantive test for determining inventorship, it is structured around the premise of human contribution, with Article 60(1) EPC vesting the right to a European patent in the inventor or

³⁰ *Trinidad v. OpenAI Inc.*, No. 25-cv-06328-JST (N.D. Cal. Jan. 5, 2026)

³¹ Victoria A. Steadman, "Drug Discovery: Collaborations between Contract Research Organizations and the Pharmaceutical Industry," *ACS Medicinal Chemistry Letters* 9, no. 7 (2018): 581, <https://doi.org/10.1021/acsmmedchemlett.8b00236>.

their successor in title, and Article 81 EPC requiring the applicant to designate an inventor. AI complicates this framework because it may become difficult to identify a human contribution to the invention.

The current position under the EPC is nevertheless clear: an AI system cannot be designated as an inventor. In J 8/20, the EPO's Legal Board of Appeal held that an inventor must be a natural person with legal capacity, so that designating the AI system "DABUS" as inventor failed to satisfy Article 81 and Rule 19(1) EPC.³² The Board also reasoned that because an AI system cannot hold or transfer legal rights, ownership of it cannot establish succession from a legally recognized inventor under Article 60(1) EPC.

A similar approach prevails outside Europe. In the United States, the Federal Circuit reached a corresponding conclusion in *Thaler v Vidal*, holding that the term "individual" in the Patent Act refers to a human being.³³ The United States Patent and Trademark Office's (USPTO) revised guidance likewise treats AI systems as tools and applies the ordinary standard of human conception rather than a separate test for AI-assisted inventions.³⁴ Consequently, using, owning, or supervising an AI system does not establish inventorship. Comparable conclusions have been reached in other jurisdictions, including Germany,³⁵ and the UK,³⁶. South Africa³⁷ remains, to date, the sole exception to this trend.

³² J 8/20 (Designation of Inventor/DABUS), Legal Board of Appeal of the European Patent Office, December 21, 2021.

³³ *Thaler v. Vidal*, 43 F.4th 1207 (Fed. Cir. 2022).

³⁴ Bundesgerichtshof [BGH] [Federal Court of Justice], decision of June 11, 2024, X ZB 5/22 (DABUS), <https://www.wipo.int/wipolex/en/judgments/details/2495>

³⁴ USPTO, *Revised Inventorship Guidance for AI-assisted Inventions* (2025)

³⁵ Bundesgerichtshof, *DABUS*.

³⁶ *Thaler v Comptroller-General of Patents, Designs and Trade Marks* [2023] UKSC 49 (December 20, 2023).

³⁷ Stephen L. Thaler, Food Container and Devices and Methods for Attracting Enhanced Attention, South African Patent No. ZA 2021/03242 (filed May 13, 2021; published July 28, 2021).

It is worth noting that while countries are broadly moving in the same direction, divergences do exist. The central question in AI-assisted R&D disputes is rarely whether a human was involved at all, but rather how much involvement, and of what kind, is legally sufficient. The United States and Europe diverge in how that question is framed. The USPTO treats AI as a tool and applies ordinary conception-based inventorship principles whereas the EPO approaches the issue through the EPC framework for inventor designation and entitlement, requiring an identifiable natural person whose contribution can be connected to the claimed technical subject matter. For applicants filing in both jurisdictions, the same research record may therefore need to support two differently framed analyses of the human role in an AI-assisted invention.³⁸

China's evolving framework adds a further layer to this picture. On inventorship, China National Intellectual Property Administration (CNIPA)'s recent amendment to the Patent Examination Guidelines aligns with both the EPO and the USPTO in substance: Rule 14 confirms that an inventor must be a natural person, and AI accordingly cannot be named as inventor on a Chinese application.³⁹ Where China appears to depart more clearly from the European and US approach is in the broader examination framework for AI-related inventions. Recent CNIPA guidance and amendments place express emphasis on legal compliance, social morality, public interest and ethical concerns in AI-related applications, alongside more detailed provisions on inventive step and sufficiency of disclosure.⁴⁰

³⁸ Jörg Smolinski, "USPTO and EPO Used to Basically Agree on AI Inventorship," LinkedIn, approx. August 13, 2026, https://www.linkedin.com/posts/j%C3%B6rg-smolinski_aipatents-patentlaw-inventorship-activity-7491384597788782592-FWr_.

³⁹ Panawell & Partners LLC, "Newly Amended Guidelines for Patent Examination to Take Effect on January 1, 2026," *Legal 500*, December 31, 2025, <https://www.legal500.com/intelligence/china/intellectual-property/newly-amended-guidelines-for-patent-examination-to-take-effect-on-january-1-2026>.

⁴⁰ "IP and AI: Pathways to Collaborative Innovation." China National Intellectual Property Administration., last updated April 30, 2025, https://english.cnipa.gov.cn/art/2025/4/30/art_3090_199446.html.

B. Practical guidance for applicants

A European patent application should therefore be supported by a coherent account of the human contribution: who formulated the technical problem; who selected or designed the approach; who imposed technically meaningful constraints on the AI system; who interpreted its outputs; who selected or modified the eventual candidate; and who recognized or experimentally established the claimed technical effect.⁴¹

In AI-assisted drug discovery, whether an individual can properly be identified as the inventor under the law will depend heavily on the facts. When a researcher merely gives a model a broad instruction to identify a compound capable of treating a disease it may be difficult to establish a sufficiently direct intellectual contribution to a subsequently generated molecule.

By contrast, a researcher may make a relevant contribution by formulating a specific technical hypothesis, defining and constraining the chemical space, selecting biologically meaningful parameters, curating or weighting training data for a particular technical purpose, setting optimization objectives, filtering outputs on technical grounds, modifying an AI-proposed structure, or recognizing that a particular output possesses an unexpected therapeutic property. The more closely the researcher's contribution is connected to the technical features of the claimed invention, the stronger the inventorship position is likely to be.

Pharmaceutical inventions often emerge through collaborative and iterative work. A model developer, data scientist, medicinal chemist, biologist and clinician may all contribute, but not every valuable contribution is inventive. Routine implementation, data generation, project management, platform ownership or general supervision may be insufficient unless they helped devise the technical features ultimately claimed. Inventorship should therefore be assessed claim by claim, by asking who contributed intellectually to the distinguishing technical features, rather than by reference to job title, seniority or the overall importance of their work.

⁴¹ Zhipeng Zhu, "Patentability of AI-Assisted Inventions: Guidance, Case Law, and a Roadmap Forward," *University of Cincinnati Intellectual Property and Computer Law Journal* 11, no. 1 (2026): 169–86, <https://scholarship.law.uc.edu/ipclj/vol11/iss1/9>.

Consequently, applicants should assess inventorship alongside claim drafting rather than treating it as a separate administrative exercise.⁴² Applicants should support that analysis with clear, contemporaneous records, lab notebooks, invention-disclosure forms, model-development logs, and similar documentation, showing: the technical problem addressed; why specific models, datasets, inputs, or parameters were chosen; the constraints and optimization objectives applied; how outputs were evaluated and ranked; what changes were made to AI-generated proposals; and which experiments proved the claimed technical effect.

Preserving evidence of the human contribution is therefore both a legal and a strategic task. The objective is to demonstrate how human expertise directed or constrained the computational process and how human judgment converted its outputs into a claimed technical solution. From a European patent-law perspective, the strongest applications will be those that make this pathway, and its connection to the claimed subject matter, visible from the outset.

IV. Sufficiency of Disclosure: Making the Technical Effect Reproducible

A. The legal standard

Sufficiency is another pressure point for AI-assisted drug discovery. The required disclosure will differ depending on whether the claim concerns an AI-discovered product or use, an AI-based method or the underlying AI technology. Article 83 and Rule 42(1)(e) EPC require an enabling technical teaching, including at least one detailed way of performing the invention, rather than a mere statement of the desired result. Patent offices generally assess AI-assisted inventions under ordinary sufficiency, enablement, support and, where applicable, best-mode requirements.

Like any other claim, a pharmaceutical product claim must be supported by the application as filed, including disclosure enabling the skilled person to make the product and evidence making the asserted therapeutic utility credible. The EPO does not impose any AI-specific duty

⁴² V. Teplitskiy, "What Inventors Need to Know about the Patentability of AI-Assisted Inventions in the United States," *IAM*, June 10, 2026, <https://www.iam-media.com/article/what-inventors-need-know-about-the-patentability-of-ai-assisted-inventions-in-the-united-states>.

to disclose the mere fact that AI was used in drug discovery or clinical development. Where the claimed product, therapeutic use or experimental result can be independently enabled and justified, background AI use will usually not require separate disclosure. By contrast, where the AI output, model, training process, input-output relationship or validation is essential to reproducing or substantiating the technical effect, non-disclosure may create prosecution or post-grant risks.

The EPO Guidelines accordingly recognize that an AI-related invention may be insufficiently disclosed where the mathematical methods and training datasets are described in insufficient detail to reproduce the technical effect without undue burden over the whole claim scope.⁴³ The Guidelines do not, however, generally require disclosure of the exact training dataset; where the technical effect depends on particular characteristics of the data, only those characteristics must be disclosed, unless the skilled person could determine them without undue burden from common general knowledge.

The technical Boards of Appeal decision T 161/18⁴⁴ shows the risk where a trained model is essential to the technical effect. The Board found the neural-network training irreproducible because the necessary input data and methodology were inadequately disclosed. General statements that data are “large,” “diverse” or “representative” may therefore be insufficient.

T 1669/21⁴⁵ confirms that Article 83 EPC does not invariably require disclosure of datasets, source code or model weights. The application must instead describe the technically relevant inputs, outputs and their relationship sufficiently to make the solution credible and

⁴³ European Patent Office, “3. Insufficient Disclosure,” in *Guidelines for Examination in the European Patent Office*, pt. F, ch. III (Munich: European Patent Office, 2026), https://www.epo.org/en/legal/guidelines-epc/2026/f_iii_3.html.

⁴⁴ “Equivalent Aortic Pressure/ARC Seibersdorf,” T 0161/18, Board of Appeal 3.5.05, European Patent Office, May 12, 2020, ECLI:EP:BA:2020:T016118.20200512, <https://www.epo.org/en/boards-of-appeal/decisions/t180161du1>.

⁴⁵ T 1669/21 (Refractory Intellectual Property GmbH & Co. KG v. Vesuvius Group S.A.), Technical Board of Appeal 3.2.03, European Patent Office, July 23, 2024, ECLI:EP:BA:2024:T166921.20240723, <https://www.epo.org/de/boards-of-appeal/decisions/t211669du1>.

reproducible. Vague references to “production data,” “sensor data” or “machine learning” may not suffice where the effect depends on a specific correlation.

Taken together, these decisions establish that if a technical effect depends on properties of the data, those properties form part of the enabling teaching unless they can be identified routinely from common general knowledge. Material information may include the source and type of data, selection criteria, the represented biological or chemical variables, measurement and labeling methods, and validation and testing procedures.

This is particularly important in the life sciences because biological and chemical datasets are highly context dependent.⁴⁶ Differences in assay conditions, patient populations, disease definitions, measurement platforms or labeling thresholds may change what a model learns. Life-sciences datasets may also be large, commercially confidential or subject to data-protection and research-ethics obligations.⁴⁷ These constraints may justify withholding individual records or patient-level information, but they do not lower the Article 83 standard. The critical distinction is between withholding the dataset itself and withholding the information needed to reproduce its technically relevant characteristics. If independently obtainable data can be selected and processed using the application's instructions, disclosure of the exact dataset may be unnecessary. If the effect depends on an inaccessible proprietary dataset and the application neither describes its essential characteristics nor teaches a reproducible alternative, the skilled person may face an undue research burden.

B. Practical guidance for applicants

Applicants should distinguish information needed to enable and support the claimed invention from details that merely record how it was made. Background AI use need not be disclosed unless material to sufficiency, support or patentability. Where the model, data or validation is central to the technical effect, however, the application should describe the

⁴⁶ Xiao, Ruyi, and Jin Zhang. “The Sufficiency of Disclosure in Medical AI Patents: Evidence from 865 Granted Patents Across the US, China, and the EU.” *Journal of Law, Medicine & Ethics*, April, 1–14 (2026): <https://doi.org/10.1017/jme.2026.10256>.

⁴⁷ Xiao and Zhang, “Sufficiency of Disclosure”

relevant inputs, outputs, process, selection criteria, validation and link to the claimed pharmaceutical effect.

Proprietary assets should be protected where possible without compromising enablement. Applicants may often describe the necessary dataset characteristics—such as sources, selection rules, assay conditions, labelling, preprocessing, quality controls and limitations—without disclosing individual records, complete datasets or model weights. If the claimed effect depends on an inaccessible dataset or process, however, the disclosure or claim scope must be adjusted.

The applicant should specify, what the input data represents, how it is collected or measured, how it is labelled or varied, what the model is trained to predict, and why the disclosed inputs plausibly correlate with the claimed output. Applicants should also preserve a stable internal record of the software, datasets, model versions, and validation work used before filing.⁴⁸

Disclosure must also balance sufficiency and inventive step. A detailed account of the AI workflow may show how the skilled person could reproduce the invention, which supports sufficiency. But the same detail may invite the argument that the claimed result followed from the routine application of known computational methods, which undermines inventive step.⁴⁹ The more the specification presents the process as a standard pipeline, the easier it is to say that the outcome was obvious.

The specification should therefore strike a balance. It should contain enough technical information for a skilled person to reproduce the invention even if the particular AI model or software version has since been replaced. It should also avoid unnecessary disclosure of commercially sensitive material, such as proprietary models, datasets, validation workflows, or discovery know-how. These may be better protected as trade secrets.

⁴⁸ Zhu, “Patentability of AI-Assisted Inventions”

⁴⁹ Ella Green, “AI and Inventive Step: Does Machine-Generated Mean Obvious? ”, *Carpmaels & Ransford*, August 3, 2026, <https://www.carpmaels.com/ai-and-inventive-step-does-machine-generated-mean-obvious-2/>

V. Inventive Step: Defining the AI-Augmented Skilled Person

A. The legal standard

Inventive step is the third major pressure point for AI-assisted drug discovery. Under Article 56 EPC, an invention involves an inventive step if it is not obvious to the skilled person in light of the prior art, and as AI tools become standard equipment in pharmaceutical research, they may shift the baseline against which inventive contribution is assessed.

Under European patent law, a large language model (LLM) is not (yet) a person skilled in the art. In T 1193/23,⁵⁰ the Board of Appeal questioned the reliability of LLM-generated interpretations of technical terms in patent claims, addressing whether output from an LLM trained on broad, undifferentiated internet data can serve as evidence of how a person skilled in the art would understand a claim term. The Board held that any such AI-derived insight must be corroborated by established technical literature or expert testimony, and it identified three limitations underlying this conclusion: LLMs are trained on data of unknown provenance and scope; their outputs are highly sensitive to how a question is framed and to its surrounding context; and their responses cannot be assumed to track the understanding of an actual skilled practitioner, particularly as of the relevant priority date. As AI use becomes more widespread, computational drug discovery may in time be absorbed into the skilled person's ordinary toolkit for routine work and experimentation, and if so, the EPO's inventive step requirements for pharmaceutical applications could become correspondingly more exacting.

1. “Could” versus “would” in AI-assisted invention

Inventive step and obviousness are assessed objectively by the EPO. The actual route by which the inventors reached the invention is generally not decisive.⁵¹ A discovery may have involved extensive effort, expensive modeling and sophisticated experimentation, but that does not by itself make the claimed subject matter inventive. Conversely, a solution generated

⁵⁰ European Patent Office, Board of Appeal 3.2.06, *Rieter CZ s.r.o. v. Saurer Spinning Solutions GmbH & Co. KG*, Case No. T 1193/23, Decision of April 15, 2025, <https://www.epo.org/de/boards-of-appeal/decisions/t231193du1>.

⁵¹ Green, “AI and Inventive Step”

quickly with the help of AI is not automatically obvious. The inquiry remains whether the notional skilled person, starting from the prior art and using common general knowledge, would have arrived at the claimed solution without inventive ingenuity.

In this context, the EPO's familiar distinction between what the skilled person *could* have done and what they *would* have done becomes particularly important. The fact that an AI system could, in principle, generate a particular compound, target, or prediction does not establish that the skilled person would have selected that tool, used it in the relevant way, trusted its output, or arrived at the claimed solution.

2. The EPO's Problem Solution Approach Applied to AI Tools

The EPO's Problem Solution Approach by and large governs how inventive step is assessed in Europe. The examiners identify the closest prior art, determine the distinguishing features of the claim, formulate the objective technical problem based on the technical effect achieved, and then ask whether the claimed solution would have been obvious to the skilled person. For AI-assisted inventions, two aspects of this framework are particularly important. First, only features that contribute to a technical effect can support inventive step. Secondly, the capabilities and ordinary tools of the skilled person must be assessed as they existed at the relevant date, which is precisely where AI complicates the analysis as the ordinary tools of the skilled person evolve over time.⁵²

The skilled person may in practice be a multidisciplinary team comprising medicinal chemists, computational scientists, and biologists. Their capabilities should not be equated with those of an omniscient system with access to all data and unlimited computing power. Nor should a confidential model or proprietary dataset automatically be treated as common general knowledge.

Even where an AI tool was publicly available or formed part of that team's ordinary toolkit, its availability does not make every output obvious. The assessment must avoid hindsight and should ask whether, at the priority date, the skilled person would have had a reasonable expectation of success rather than a merely speculative prospect. It should also

⁵² Green, "AI and Inventive Step"

consider whether the claimed result produced an unexpected technical effect. This is especially important in drug discovery, where an AI-generated prediction may point to a possible protein structure, epitope, compound, or biological target, but will not necessarily provide a reliable basis for expecting that the approach will work in practice. AI outputs may therefore be treated much like other *in silico* evidence: potentially relevant, but often insufficient on their own without biological plausibility and experimental validation.

This issue is particularly acute in antibody and biologics cases, where EPO practice treats the generation of alternative antibodies to a known antigen using established techniques as potentially routine⁵³. Generative design may therefore strengthen an obviousness argument where the prior art provided a reason to seek further antibodies, the relevant AI tool formed part of the skilled person's ordinary toolkit and there was a reasonable expectation of obtaining antibodies with the claimed properties. However, the ability to generate or search a larger candidate pool should not determine the analysis by itself. Routine candidate generation does not necessarily establish a reasonable expectation of obtaining the claimed functional or therapeutic property. Nor does it necessarily enable the skilled person to obtain qualifying embodiments across the full breadth of a functional claim. The more precise question is which part of the workflow was routine at the priority date: generating candidates, identifying individual qualifying hits, or reliably obtaining embodiments across the breadth claimed.⁵⁴

B. Practical guidance for applicants

Applicants should build the inventive-step argument around a technical effect, explaining why the chosen input representation, constraints, model configuration, compound or therapeutic use provides an advantage over the prior art. The focus is whether the claimed subject matter was obvious, not the research effort invested or the sophistication of the AI tool.

⁵³ Per Larsen, "When AI Designs the Antibody, 'Routine' Lowers the Bar for Sufficiency and Raises It for Inventive Step," *AERA*, August 13, 2026, <https://aera-ip.com/when-ai-designs-the-antibody/>

⁵⁴ Larsen, "When AI Designs the Antibody"

The data used to train, fine-tune and validate pharmaceutical AI models may be as important as the model itself. Proprietary datasets may include chemical structures and structure–activity relationships, assay results, toxicity and off-target findings, pharmacokinetic and pharmacodynamic data, failed experiments, patient-derived data and clinical outcomes. Their quality, curation and combination can materially affect the candidates identified and properties predicted.

Companies should protect these assets through confidentiality, access controls, trade-secret measures and contractual restrictions, while keeping contemporaneous records of data provenance, selection, labelling, curation and validation. Such records may help show that the result arose not from routine use of a public model and data, but from technically meaningful choices and a data asset unavailable to the skilled person at the priority date.

Confidential data does not itself establish inventive step. The patent case must still identify a non-obvious claimed feature and a credible technical effect. Properly documented, however, proprietary data may support the argument that the skilled person lacked the same starting point, would not have followed the same route with a reasonable expectation of success, and could not readily have obtained the same result.

Where possible, applicants should include comparative data against the closest alternatives, identifying unexpected properties such as improved potency, selectivity, toxicity profile, stability, bioavailability or manufacturability. They should explain why the prior art would not have led the skilled team to the same solution with a reasonable expectation of success. Evidence that the model’s output required non-routine human selection, modification, interpretation or experimentation can strengthen the case, particularly where the claimed path involved technical choices not suggested by the prior art.

AI use should be described strategically. Where the invention relied on in-house or specialized tools not routinely available at the priority date, applicants should preserve evidence of their limited availability and the technical choices involved. Where public models were used, the application and supporting records should emphasize non-standard elements of the workflow, such as unusual inputs, meaningful constraints, bespoke validation or selective interpretation of outputs.

Applicants should avoid framing the invention as merely using AI to generate a molecule or antibody. Where the contribution lies in a demonstrated functional or therapeutic property, the application should explain why that property was not reasonably expected and support it across the claim's full breadth. Functionally defined claims should also disclose a reliable route to further qualifying embodiments, not merely many computational candidates or a few verified hits.

Prior-art searches should cover both the pharmaceutical subject matter and the computational technique. Applicants should record which AI tools and datasets were publicly available at the priority date, their conventional uses and limitations. Claim sets should separate the potentially protectable contributions: the compound, medical use, screening or optimization method, technical system and, where appropriate, narrower validated embodiments.

Applicants should preserve evidence of the closest prior art, why the skilled person would not have used the AI tool in the claimed way or selected its output with a reasonable expectation of success, which technical choices were non-routine, and which experimental results demonstrate an unexpected or advantageous effect.

VI. Patentability of the AI System Itself

A further question arises where protection is sought for the AI system itself: the model, algorithm, training method, or computational workflow that generated or selected the output. In AI-assisted drug discovery, commercial protection typically centers on the molecule, antibody, use, or screening method; but supplementary protection for the underlying computational method can be valuable where the model itself delivers a reproducible technical advantage, for instance, by improving the reliability of active-compound identification or reducing false positives within a technically defined screening process.

Across Europe, the United Kingdom, and the United States, AI-related inventions are not excluded merely because they involve artificial intelligence, but the claim must do more than recite an abstract model implemented on a computer.

The EPO treats artificial intelligence and machine learning as computational models and algorithms of an abstract mathematical nature, and therefore not patentable as such.⁵⁵ The first hurdle is eligibility: a claim directed to a method involving technical means, such as a computer, or to a device, will normally possess technical character as a whole and escape exclusion under Article 52 EPC. The more demanding hurdle is inventive step. For mixed claims combining technical and non-technical features, the COMVIK approach confines the assessment to those features contributing to technical character.⁵⁶ Where the claimed technical effect depends on particular characteristics of the training data, moreover, the application must disclose those characteristics sufficiently for the skilled person to reproduce the effect without undue burden.

The UK position has moved closer to the European approach. Following the Supreme Court's decision in *Emotional Perception*⁵⁷ and the UK IPO's subsequent interim guidance, the former *Aerotel*⁵⁸ framework has been shifted for computer-implemented inventions: the initial eligibility threshold is now lower where the claim involves technical means. This does not render AI inventions automatically patentable, however, a filtering exercise remains necessary so that novelty and inventive step focus on the features making a genuine technical contribution.⁵⁹

⁵⁵ “Mathematical Methods”, Examination Guideline, European Patent Office, accessed October 14, 2026, https://www.epo.org/en/legal/guidelines-epc/2026/g_ii_3_3.html

⁵⁶ “9.2.1 The Comvik Approach,” in *Case Law of the Boards of Appeal of the European Patent Office*, 2025 ed., I. Patentability, D. Inventive Step, 9. Assessment of Inventive Step, 9.2. Problem-and-Solution Approach When Applied to Mixed-Type Inventions,” European Patent Office, accessed August 28, 2026, https://www.epo.org/en/legal/case-law/2025/clr_id_9_2_1.html.

⁵⁷ *Emotional Perception AI Ltd v Comptroller General of Patents, Designs and Trade Marks* [2026] UKSC 3, <https://supremecourt.uk/cases/uksc-2024-0131>

⁵⁸ “Supreme Court Overrules *Aerotel* and Aligns UK Approach to AI and Computer-Implemented Inventions with the EPO,” *Herbert Smith Freehills Kramer*, February 11, 2026, <https://www.hsfkramer.com/notes/ip/2026-02/supreme-court-overrules-aerotel-and-aligns-uk-approach-to-ai-and-computer-implemented-inventions-with-the-epo>.

⁵⁹ Kate Harkness, “Interim Guidance from the UK IPO on Computer-Implemented Inventions,” *Murgitroyd*, April 7, 2026, updated April 10, 2026,

In the United States, the USPTO's 2024 AI subject-matter eligibility update likewise creates no AI-specific test;⁶⁰ AI claims are assessed under the ordinary § 101 framework. The governing questions are whether the claim recites an abstract idea and, if so, whether that idea is integrated into a practical application, for example, by improving the functioning of a computer or another technology or technical field. Merely applying an AI model on a generic computer, confining an abstract idea to a particular field of use, or appending insignificant extra-solution activity will generally not suffice. The USPTO's AI Examples 47–49 illustrate the same principle: eligibility turns on whether the claim is tied to a practical technological application, not on the fact that AI is used.

A drug-discovery example illustrates the distinction. A claim to "using a neural network to identify drug candidates for treating fibrosis" would be vulnerable in all three jurisdictions if it merely describes an abstract prediction implemented on a computer. A claim directed to a technically defined screening method, by contrast, stands on firmer ground where it specifies the relevant molecular representations, model architecture or training constraints, the biological or chemical input data, the selection thresholds, and the experimental validation linking selected compounds to an improved technical effect, such as increased target selectivity or reduced toxicity.

VII. Regulatory Requirements

Patent strategy should account for the evolving pharmaceutical regulatory framework. In January 2025, the US Food and Drug Administration (FDA) issued draft guidance setting out a risk-based framework for the use of AI models to generate information or data supporting regulatory decision-making on the safety, effectiveness or quality of drugs and biological

<https://www.murgitroyd.com/insights/patents/interim-guidance-from-the-uk-ipo-on-computer-implemented-inventions>.

⁶⁰ “USPTO Issues AI Subject Matter Eligibility Guidance,” *U.S. Patent and Trademark Office*, July 16, 2024, <https://www.uspto.gov/subscription-center/2024/uspto-issues-ai-subject-matter-eligibility-guidance>.

products.⁶¹ Although it excludes preclinical discovery before regulatory engagement, it covers downstream applications such as pharmacokinetic, pharmacodynamic and toxicological modelling and predictive dose selection.

The framework emphasizes methodological transparency. Training-data quality, size and representativeness may introduce bias and affect output reliability. Depending on the model, its intended use and risk, companies may need to disclose data collection and controls, dataset selection and labelling, inputs and outputs, architecture, feature selection, hyperparameters and pretrained components. The extent required will reflect the model's risk and the importance of its output to the regulatory decision.

The FDA's draft guidance is part of a broader international response to the growing use of AI in pharmaceutical development.⁶² In September 2024, the European Medicines Agency (EMA) finalized its *Reflection Paper on the Use of Artificial Intelligence in the Medicinal Product Lifecycle*.⁶³ The paper identifies potential benefits and risks in the use of AI in drug discovery and emphasizes transparency, validation, human oversight and good practice throughout the medicinal-product lifecycle. In the United Kingdom, the Medicines and Healthcare products Regulatory Agency has likewise issued guidance concerning AI in medical devices and other health products.⁶⁴ The FDA has addressed AI-enabled medical devices

⁶¹ U.S. Food and Drug Administration, "Considerations for the Use of Artificial Intelligence To Support Regulatory Decision-Making for Drug and Biological Products," Draft Guidance for Industry and Other Interested Parties, 2025, <https://www.fda.gov/regulatory-information/search-fda-guidance-documents/considerations-use-artificial-intelligence-support-regulatory-decision-making-drug-and-biological>.

⁶² "FDA Draft Guidance on AI in Drug Development Explained," *IntuitionLabs*, April 1, 2026, <https://intuitionlabs.ai/articles/fda-draft-guidance-ai-drug-development>.

⁶³ Hester Borgers, "EMA's Finalised Reflection Paper on the Use of AI," *TwoBirds*, January 22, 2025, <https://biotalk.twobirds.com/post/102juyw/emas-finalised-reflection-paper-on-the-use-of-ai>.

⁶⁴ "Software and Artificial Intelligence (AI) as a Medical Device," UK Government, last updated February 3, 2025, <https://www.gov.uk/government/publications/software-and-artificial-intelligence-ai-as-a-medical-device/software-and-artificial-intelligence-ai-as-a-medical-device>.

through a separate regulatory framework and issued related draft guidance on the same day as its guidance on AI supporting drug and biological-product submissions in early January 2025.⁶⁵ Together, these developments show AI being incorporated into the regulatory oversight of medicinal products.

The FDA and EMA approaches are not identical. The FDA focuses more specifically on the credibility and risk of models used in regulatory decision-making, whereas the EMA addresses principles and good practice across the whole medicinal-product lifecycle. Both, however, emphasize risk assessment, transparency and validation, and their parallel development may encourage greater international alignment.

These developments matter for patent strategy because regulatory submissions may increasingly require more detailed about AI systems than patent applications do.⁶⁶ Innovators should expect AI methods, evidence and limitations to be compared across patent applications, regulatory submissions and publicrecords. Material inconsistencies could undermine the credibility of the evidence, raise questions about sufficiency or inventorship, or weaken prosecution or enforcement positions.

Regulatory disclosures on model reliability, data limitations, validation failures, uncertainty or candidate selection may later be read as admissions that the workflow was routine, the technical effect uncertain at filing, or predictive value dependent on undisclosed data. Patent and regulatory teams should therefore align terminology, evidence and explanations of AI performance before positions enter public or regulatory records.

⁶⁵ U.S. Food and Drug Administration, "Artificial Intelligence-Enabled Device Software Functions: Lifecycle Management and Marketing Submission Recommendations," Draft Guidance for Industry and Food and Drug Administration Staff, January 2025, <https://www.fda.gov/regulatory-information/search-fda-guidance-documents/artificial-intelligence-enabled-device-software-functions-lifecycle-management-and-marketing>.

⁶⁶ Bruno Quinney, "Legal Issues Arising from the Use of Artificial Intelligence in Drug Development," *Drug Discovery World (DDW)*, February 11, 2026, <https://www.ddw-online.com/legal-issuesvdrug-development-40410-202602/>.

VIII. Improving Legal Certainty

The preceding analysis demonstrates that AI-assisted drug discovery does not require patent law to abandon its established principles. The existing doctrines of human inventorship, sufficiency of disclosure and inventive step remain capable of accommodating inventions developed with the assistance of AI. The principal policy challenge is therefore not the absence of an applicable legal framework, but the increasing factual complexity and uncertainty involved in applying that framework.

Drug development requires substantial investment, involves long development timelines and remains subject to considerable technical and regulatory risk.⁶⁷ Bringing a single compound to market often takes more than a decade and billions of dollars. Companies, universities and investors consequently need a reasonable degree of predictability as to whether AI-assisted discoveries can be adequately protected. Generative AI may compress discovery tasks, including virtual screening, target prioritization and molecule optimization. A systematic review of 100 studies published between 2018 and 2025 reports its greatest impact in early-stage discovery, where timelines for molecule identification and lead optimization shortened and experimental costs fell.⁶⁸

Much of that evidence, however, rests on in-silico proof-of-concept studies, and evidence of reduced time or cost at those stages should not be conflated with elimination of downstream development risk. In preclinical development, applications remain limited and prospective validation is sparse. In clinical development, the gains are primarily in cost rather than time, and there is no robust evidence yet that computational acceleration translates into reduced attrition or regulatory progress.⁶⁹ The extent of any cost saving therefore remains method- and

⁶⁷ Xie et al., “AI in Drug Development.”

⁶⁸ Aaron Riemer and Victoria Freund, “Generative Artificial Intelligence in Pharmaceutical Drug Development: A Systematic Review of Time and Cost Efficiency across Discovery, Preclinical, and Clinical Phases,” *Intelligent Pharmacy* 4, no. 2 (April 2026): 145, <https://www.sciencedirect.com/science/article/pii/S2949866X25000784>.

⁶⁹ Duxin Sun and Christian Macedonia, “Will AI Revolutionize Drug Development? Researchers Explain Why It Depends on How It’s Used,” *Journal of Health Economics and*

program-specific, and the review also identifies hidden costs and methodological, regulatory and ethical barriers. Clinical validation, manufacturing and regulatory review continue after candidate selection.

An appropriate policy response should balance two competing risks. If AI-assisted discoveries are too difficult to protect, innovators may rely more heavily on trade secrecy, thereby reducing disclosure and limiting cumulative innovation. Conversely, granting broad protection on the basis of opaque computational predictions could restrict follow-on research and competitive market entry without securing a commensurate technical contribution. Patent policy should therefore preserve incentives for genuine and sufficiently disclosed innovation while preventing claims that extend beyond what the applicant has plausibly demonstrated.

This raises a wider policy question. If AI makes some stages of candidate generation cheaper or faster (a proposition that is still debated),⁷⁰ the case for exclusivity cannot rest simply on the amount of discovery effort expended. The traditional justification, that patents incentivise/reward costly and uncertain research, carries less weight if that part of the process becomes less costly. However, lower discovery costs do not remove the substantial cost, delay and risk of the later stages: preclinical development, clinical testing, and regulatory approval. Patent rights may therefore remain important as transactional assets, supporting financing, enabling licensing, and allocating those downstream risks between parties. The policy question is therefore whether the claimed technical contribution justifies the scope of exclusivity sought. The test should not revolve around the use of AI nor the historical cost of R&D, but what the applicant has contributed technically and whether the breadth of the claim is proportionate to it.

The tradeoff plays out differently depending on the method. Where a generative model proposes candidate molecules that are then synthesized and tested, the validated compound

Outcomes Research, January 3, 2025, <https://jheor.org/post/2904-will-ai-revolutionize-drug-development-researchers-explain-why-it-depends-on-how-it-s-used>.

⁷⁰ Aaron Riemer and Victoria Freund, “Generative Artificial Intelligence in Pharmaceutical Drug Development: A Systematic Review of Time and Cost Efficiency across Discovery, Preclinical, and Clinical Phases,” *Intelligent Pharmacy* 4, no. 2 (April 2026): 145, <https://www.sciencedirect.com/science/article/pii/S2949866X25000784>.

supplies a concrete anchor for a patent claim. Where a model only ranks targets or predicts binding in silico, the output is closer to an untested prediction, and broad claims built on it risk exceeding what has actually been shown. In the first case the main concern is adequate disclosure of how the model contributed. In the second it is claim scope.

The balance also differs by layer of the AI-biopharma ecosystem. A platform provider may depend principally on trade secrets and contract-based control over training data, model access and permitted downstream use. A drug developer may depend more heavily on patents covering a validated molecule or therapeutic use. Collaborators may use contractual allocation of rights in inputs, outputs and validation data as a de facto mechanism for controlling commercially valuable information that patent law does not itself protect.⁷¹ Such contractual rights can support investment and transaction, but, because they bind the parties rather than the public at large, they should not be treated as a substitute for satisfying patentability requirements.

A. Preserve technology-neutral principles

The primary policy objective should be to improve legal certainty without premature legislative intervention. There is presently no compelling need to create a separate category of patent rights for AI-generated inventions or to recognize AI systems as inventors. Either reform would generate substantial questions concerning ownership, entitlement, legal responsibility and compatibility with international patent systems.⁷²

A more proportionate approach is to clarify how established patent doctrines apply when AI forms part of the inventive process. This would preserve the technology-neutral character of the patent system while allowing its principles to respond to changes in research practice.

⁷¹ De Werra, Jacques. “Intellectual Property Transactions: What We Can (and Should) Learn from Contract Law for IP Licensing.” *GRUR International* 69, no. 11 (November 2020): 1095-96. <https://doi.org/10.1093/grurint/ikaa137>.

⁷² Aboy, Mateo, and Kathleen Liddell. “United States Patent and Trademark Off Ice.” *Journal of Intellectual Property Law & Practice* 21 (5): 54636–37 (2026). <https://doi.org/10.1093/jiplp/jpag021>.

AI involvement should be neither a ground for preferential treatment nor a basis for excluding an otherwise patentable invention.

Accordingly, the patentability threshold should not be lowered merely because an output was generated with AI. Such an approach could confer exclusive rights over results obtained through routine computational screening. Equally, an invention should not be denied protection simply because an AI system made a substantial contribution to its development. The decisive questions should remain whether the statutory requirements have been satisfied and whether the claimed invention reflects a genuine, sufficiently disclosed technical contribution.

B. Clarify human inventorship

Patent offices should provide consolidated, claim-specific examples of the contributions that may support inventorship in AI-assisted research. Such guidance should also make clear that merely owning, operating or commissioning an AI system will not necessarily establish inventorship. The relevant inquiry is whether a natural person made an intellectually significant contribution to the subject matter of the particular claim.

More autonomous forms of agentic AI may eventually test the limits of this framework.⁷³ Nevertheless, it would be premature to resolve hypothetical cases by automatically attributing an AI-generated invention to the system's developer, owner or user. Attribution without a corresponding inventive contribution would sit uneasily with existing inventorship principles. If AI systems ultimately acquire a legally relevant degree of autonomy, the issue may need to be considered alongside broader questions of legal personality, capacity, ownership and responsibility. Until a genuine protection gap is demonstrated, policy should concentrate on documenting and evaluating human contributions more effectively.

C. Define the AI-augmented skilled person realistically

Inventive step should reflect the tools realistically available to the skilled person at the priority date. An AI system's ability to generate a candidate does not establish that the skilled

⁷³ Aboy and Liddell, "USPTO Ice"

person would have selected that tool, provided the necessary inputs, followed the same pathway or reasonably expected success.

However, publicly accessible and commonly used models, datasets or methods suitable for the task and capable of reasonably predictable results may form part of the skilled person's ordinary toolkit. Patent offices and courts should therefore assess the AI-augmented skilled person realistically and at the relevant date, considering tool and data availability, routine use, the prior art's reason to use them, any technically significant choices and the reasonable expectation of success. In pharmaceuticals, computational identification of a molecule or target should not alone establish obviousness, given the uncertainty in translating *in silico* predictions into credible biological or therapeutic effects.

D. Set proportionate disclosure expectations

Greater clarity is also needed regarding the disclosure of AI-assisted inventions. The governing question should remain whether the patent enables the skilled person to perform the claimed invention across its scope, rather than whether the AI tools used to arrive at that invention are disclosed for their own sake. On this basis, there should be no automatic requirement to disclose source code, complete training datasets or model weights whenever AI has been used. Such information may simply be irrelevant where the claimed technical effect can be reproduced from the disclosed compounds, experimental procedures and validation data.

The position changes, however, where the operation or performance of the AI system is itself essential to reproducing the claimed effect; in such cases, more detailed information becomes necessary. Depending on the invention, this may include the model architecture, training methodology, material characteristics of the dataset, input representation, optimization criteria, validation procedures and the relationship between computational predictions and experimental results. Because the appropriate level of disclosure will vary case by case, patent offices should issue guidance identifying the information normally required in different factual circumstances and should encourage the use of recognized reporting standards to promote consistency.⁷⁴

⁷⁴ Xiao and Zhang, "Sufficiency of Disclosure"

For example, if a patent claims a specific molecule and provides conventional synthesis and assay data sufficient to establish its therapeutic effect, the undisclosed generative model that first suggested the molecule may be historically interesting but unnecessary for reproduction. By contrast, if the claim is to an AI-based screening method whose asserted reduction in false positive depends on a particular molecular representation, training population and decision threshold, those features may form part of the enabling teaching because a skilled person cannot reproduce the claimed performance without them.

Even a clearer disclosure standard, however, is only as effective as the system's capacity to apply it consistently. Examination practice has traditionally focused on novelty and inventive step, while sufficiency has received comparatively less attention.⁷⁵ As Xiao and Zhang suggest, addressing this imbalance at its root requires reinforcing examination capacity itself.⁷⁶ This means ensuring that patent examiners receive targeted training in AI methodologies, dataset limitations, validation techniques and the relationship between computational predictions and experimental evidence. In technically complex cases, access to specialist expertise, such as an "AI expert consultation pool",⁷⁷ may also improve the assessment of whether an application provides a genuinely enabling disclosure.⁷⁸

E. Coordinate internationally

The European Patent Office should develop consolidated, example-based guidance addressing AI-assisted invention under the existing provisions of the European Patent Convention. Sector-specific examples for drug discovery would be especially valuable. They should cover claim-specific human contributions relevant to inventorship; the disclosure of

⁷⁵ Michael D. Frakes and Melissa F. Wasserman, "Is the Time Allocated to Review Patent Applications Inducing Examiners to Grant Invalid Patents? Evidence from Microlevel Application Data," *Review of Economics and Statistics* 99, no. 3 (2017): 552, https://doi.org/10.1162/REST_a_00605.

⁷⁶ Xiao and Zhang, "Sufficiency of Disclosure"

⁷⁷ S. Sean Tu and Christopher M. Holman, "Antibody Patents: Use of the Written Description and Enablement Requirements at the Patent & Trademark Office," *Berkeley Technology Law Journal* 38, no. 1 (2023): 33–39.

⁷⁸ Xiao and Zhang, "Sufficiency of Disclosure"

models, data and computational methods; the evidence required to support predicted therapeutic effects; the treatment of routine and specialized AI tools under the problem–solution approach; and the distinction between computationally generated candidates and experimentally substantiated technical effects.

The purpose of such guidance should not be to create separate AI-specific patentability tests. It should instead promote the consistent application of existing principles by applicants, examiners and courts.

International coordination is equally important. Pharmaceutical inventions are commonly prosecuted, licensed and enforced across Europe, the United States, China, Japan, Korea and other major markets, yet a meaningful divergence has already emerged between the European and US approaches to assessing a human's role in AI-assisted invention, as noted above.

Divergent approaches to inventorship, disclosure and inventive step increase prosecution costs, complicate global filing strategies and create avoidable uncertainty for licensing and investment. At present, the EPO, WIPO and national patent offices should therefore work toward compatible principles and drafting practices.

IX. Conclusion

This article asks whether Europe's patent framework can accommodate pharmaceutical innovation in which AI contributes materially to the inventive process. It argues that it can, provided applicants substantiate a natural person's intellectually significant contribution to the claimed technical features, disclose enough to make the technical effect reproducible, and assess inventive step against the AI tools realistically available at the priority date. The EPC's core doctrines are sufficiently flexible, but their application requires greater factual precision and more consistent guidance.

Relevant contributions may include formulating a technical hypothesis, defining meaningful constraints or inputs, modifying an AI-generated proposal, or recognising and experimentally establishing an output's technical significance; mere ownership, operation or general supervision should not suffice. Because these activities form a continuum, similar workflows may be characterised differently. Example-based patent-office guidance should

therefore focus on the link between the human act and the claimed features, rather than a quantitative threshold for human involvement.

That flexibility should not be mistaken for certainty. Questions remain about the boundary between Article 83 EPC and trade-secret protection; whether routine AI-assisted candidate generation enables or renders obvious the breadth of antibody and biologics claims; and how disclosures under the FDA's 2025 draft guidance and the EMA's Reflection Paper may affect patent-prosecution positions. These reflect the difficulty of applying settled principles to a maturing technology.

The central challenge is not whether AI-assisted inventions can be patented in Europe, but whether the patent system can convert genuine technical contributions into predictable, enforceable rights as the boundary between human and machine input becomes harder to identify and prove. Greater patent-office clarity, careful applicant documentation and closer international coordination will be needed to preserve that function.