

Artificial intelligence, drug discovery and the disclosure requirement in patent law

Abstract:

The transition from traditional to AI-driven drug discovery is transforming pharmaceutical research. Companies increasingly rely on machine learning and deep learning systems to accelerate the identification and optimisation of therapeutic candidates. This technological shift places renewed pressure on the legal framework governing patent disclosure. Under Article 83 EPC, the patent bargain requires applicants to disclose their inventions clearly and completely enough for a skilled person to reproduce them without undue burden. In the pharmaceutical sector, this has traditionally involved providing empirical evidence that a claimed compound plausibly achieves its therapeutic effect. However, AI-driven discovery often generates candidate molecules before any wet-lab validation exists, raising the question of whether in silico data alone can satisfy the sufficiency-of-disclosure requirement. A further challenge concerns whether applicants must disclose the AI models or training data used to generate such candidates. This article contributes to the emerging debate by re-examining sufficiency of disclosure for AI-driven drug inventions under European patent law. It pursues two objectives: first, to clarify how current disclosure standards are interpreted and applied to AI-driven pharmaceutical inventions; and second, to assess whether these standards remain fit for purpose in an era of increasingly data-driven and computational drug discovery. The article offers policy-oriented reflections on how European patent law can balance incentives for innovation with safeguards against overly broad or speculative claims. It concludes with a practical guidance for practitioners drafting and prosecuting patent applications in the field of AI-driven drug discovery.

Keywords: Patents; sufficiency of disclosure; drug-discovery; European law; policy; in silico data.

1. *The promise of AI in healthcare: fiction or reality?*

Bringing a new drug to market has traditionally been a complex process in the pharmaceutical industry.¹ Identifying new molecules (or new uses for known molecules) to treat a given human disease-related condition is often a time-consuming and expensive process. It might take up to 20 years to bring a new drug to the market.² The drug discovery phase process itself usually takes between 5 to 6 years.³ This process screens millions of chemical compounds to identify those that can act on disease-related targets and produce the desired therapeutic effects. Although thousands of compounds may be assessed, only a small fraction demonstrate sufficient promise to warrant further investigation. Estimates suggest that out of approximately 10,000 compounds screened during discovery, only 10–20 advance to the development phase, and roughly half of these proceed to preclinical testing.⁴

Within the drug discovery domain, antibodies are unique.⁵ They are widely used as essential tools in molecular biology research and form the basis of many diagnostic tests. For instance, they are used in vaccine-induced immunity against COVID-19.⁶ An antibody is a protein produced by the immune system in response to a foreign substance (also known as an antigen). Antibodies are made of small building blocks called amino acids. Each antibody recognises or “binds” to a specific antigen or “target” and prevents it from performing its normal biological role in the disease process.⁷ Their ability to recognise antigens with high specificity makes antibodies particularly relevant in therapeutic, diagnostic, and biotechnological contexts.⁸ However, the whole process of antibody discovery, i.e. determining if an antibody has the desired characteristics in terms of binding to the antigen, rests on trial-and-error observation.⁹ This is because each amino acid has its own chemical properties, and the order in which

¹ Natesh Singh et al., *Drug Discovery and Development: Introduction to the General Public and Patient Groups*, 3 FRONT. DRUG DISCOV. 1 (2023) (noting that “Providing efficient and safe drug to patients is a long and complex process.”).

² Boston Consulting Group, *Unlocking the potential of AI in drug discovery* (London: Wellcome Trust, 2023); <https://wellcome.org/reports/unlocking-potential-ai-drug-discovery>; Hughes JP, Rees S, Kalindjian SB, Philpott KL. Principles of early drug discovery. *Br J Pharmacol.* 2011 Mar;162(6):1239-49. doi: 10.1111/j.1476-5381.2010.01127.x. PMID: 21091654; PMCID: PMC3058157. See also: European Commission, *European Data Market Study 2024-2026. Story 2- Data Driven Innovation and Drug Discovery Disruption*. Available at: (https://ec.europa.eu/newsroom/repository/document/2024-47/Story_2_data-driven_innovation_and_drug_discovery_FINAL_)

³ See: *Drug Discovery Process*, Available at < <https://www.ppd.com/what-is-a-cro/drug-discovery-and-development/> > Last accessed 11 December 2025.

⁴ *The Pharmaceutical Journal*, Drug development: the journey of a medicine from lab to shelf; Online:DOI:10.1211/PJ.2015.20068196. <https://pharmaceutical-journal.com/article/feature/drug-development-the-journey-of-a-medicine-from-lab-to-shelf>

⁵ Lemley, Mark A. and Sherkow, Jacob S., *The Antibody Patent Paradox* (February 28, 2023). 132 *Yale Law Journal* 994 (2023), University of Illinois College of Law Legal Studies Research Paper No. 22-26, Available at SSRN: <https://ssrn.com/abstract=4032912> or <http://dx.doi.org/10.2139/ssrn.4032912>; <https://synapse.patsnap.com/article/what-are-antibodies-used-for-in-drug-development?>

⁶ *Ibid.*

⁷ See: Para §9-17, UPC Decision of the Court of Appeal of 25 November 2025, *Sanofi v Amgen*, UPC_CoA_529/2024 and CFI UPC_CoA_528/2024.

⁸ Because antibodies are so specific to their targets, they are increasingly preferred, in many therapeutic contexts, over older, “small molecule” drugs that might have unwanted side effects on other body systems. See: Kohzoh Imai & Akinori Takaoka, *Comparing Antibody and Small-Molecule Therapies for Cancer*, 6 *NATURE REV. CANCER* 714, 722-23 (2006) (comparing adverse events in small molecule drugs versus monoclonal-antibody therapies).

⁹ See: Para §9-13, UPC Decision of the Court of Appeal of 25 November 2025, *Sanofi v Amgen*, UPC_CoA_529/2024 and CFI UPC_CoA_528/2024. For instance, in *Amgen v. Sanofi*, the Court’s decision rested, at least in part, on the inability of scientists to predict which amino acid sequences would produce three-dimensional shapes with the desired characteristics.

they are arranged determines how the antibody folds into a three-dimensional shape. This shape controls which target molecules the antibody can bind to and how it works in the body.¹⁰

Pharmaceutical companies invest billions of dollars in research, clinical trials, and regulatory approvals, yet only a small percentage of drugs ever reach patients. Drug development of both small molecules and antibodies is highly expensive. Recent studies estimate that pharmaceutical companies may spend between 150 million and over 4 billion USD across the overall process of bringing a new drug to market.¹¹ Within this total, the discovery phase accounts for a smaller yet non-negligible proportion of overall research and development (R&D) expenditure. Costs are estimated at 50-300 million USD per successful drug. They depend on the number of compounds screened, the complexity and novelty of the biological target, and the technologies employed, such as high-throughput screening or biologics platforms.¹²

Therefore, drug discovery is costly and prone to high failure rates.¹³ If this process were streamlined and improved, society would benefit. This is precisely the promise of generative Artificial Intelligence (AI).¹⁴ In this paradigm shift from traditional to AI-driven drug discovery, companies use AI systems, including machine learning (ML) and deep learning (DL) algorithms, to streamline the drug discovery process.¹⁵ These systems identify potential drug targets quickly, optimise lead compounds by predicting biological activity and safety, and repurpose existing drugs for new uses.¹⁶ For instance, in 2022, Insilico Medicine announced that it used its Pharma.AI™ platform to develop an anti-fibrotic drug.

¹⁰ Lemley, Mark A. and Sherkow, Jacob S., The Antibody Patent Paradox (February 28, 2023). 132 Yale Law Journal 994 (2023), University of Illinois College of Law Legal Studies Research Paper No. 22-26, Available at SSRN: <https://ssrn.com/abstract=4032912> or <http://dx.doi.org/10.2139/ssrn.4032912>;

¹¹ Schlender M, Hernandez-Villafuerte K, Cheng CY, Mestre-Ferrandiz J, Baumann M. How Much Does It Cost to Research and Develop a New Drug? A Systematic Review and Assessment. *Pharmacoeconomics*. 2021 Nov;39(11):1243-1269. doi: 10.1007/s40273-021-01065-y. Epub 2021 Aug 9. PMID: 34368939; PMCID: PMC8516790.

¹² Ibid.

¹³ Other estimates suggest that Approximately 86% of drug candidates developed between 2000 and 2015 have failed to meet the planned target. See: <https://www.economist.com/technology-quarterly/2024/03/27/artificial-intelligence-is-taking-over-drug-development>.

¹⁴ Nic Fleming, "How artificial intelligence is changing drug discovery," *Nature*, vol. 557, no. 7707, pp. S55–S57, May 2018, doi: 10.1038/d41586-018-05267-x.; Wellcome Trust and Boston Consulting Group, *Unlocking the potential of AI in drug discovery* (London: Wellcome Trust, 2023); <https://wellcome.org/reports/unlocking-potential-ai-drug-discovery>.

<https://www.economist.com/technology-quarterly/2024/03/27/artificial-intelligence-is-taking-over-drug-development>; Debleena Paul, Gaurav Sanap, Snehal Shenoy, Dnyaneshwar Kalyane, Kiran Kalia and Rakesh K. Tekade (2021). Artificial intelligence in drug discovery and development. *Drug discovery today*, 26(1), 80–93. <https://doi.org/10.1016/j.drudis.2020.10.010>.

¹⁵ The AI Act defines AI systems as: "a machine-based system that is designed to operate with varying levels of autonomy that may exhibit adaptiveness after deployment, and that, for explicit or implicit objectives, infers, from the input it receives, how to generate outputs such as predictions, content, recommendations, or decisions that can influence physical or virtual environments." Article 3(1), Regulation (EU) 2024/1689 of the European Parliament and of the Council of 13 June 2024 laying down harmonised rules on artificial intelligence and amending Regulations (EC) No 300/2008, (EU) No 167/2013, (EU) No 168/2013, (EU) 2018/858, (EU) 2018/1139 and (EU) 2019/2144 and Directives 2014/90/EU, (EU) 2016/797 and (EU) 2020/1828 (Artificial Intelligence Act) (Text with EEA relevance) PE/24/2024/REV/1, OJ L, 2024/1689, 12.7.2024, ELI: <http://data.europa.eu/eli/reg/2024/1689/oj>. See also: Karim A.M, Artificial Intelligence in the Artificial Intelligence Act, 4iP Council (September 2025). Available at < https://www.4ipcouncil.com/application/files/4217/5740/4438/AI_in_the_EU_AI_Act.pdf >. Last Accessed 15 December 2025.

¹⁶ Sumathi S, Suganya K, Swathi K, Sudha B, Poornima A, Varghese CA, Aswathy R. A Review on Deep Learning-driven Drug Discovery: Strategies, Tools and Applications. *Curr Pharm Des*. 2023 May 19;29(13):1013-1025. doi: 10.2174/1381612829666230412084137. PMID: 37055908.; Sarkar C, Das B, Rawat VS, Wahlang JB, Nongpiur A, Tiewsoh I, Lyngdoh NM, Das D, Bidarolli M, Sony HT. Artificial Intelligence and Machine Learning Technology Driven Modern Drug Discovery and Development. *Int J Mol Sci*. 2023 Jan 19;24(3):2026. doi: 10.3390/ijms24032026. PMID: 36768346; PMCID: PMC9916967.

The drug had advanced to Phase I clinical trials roughly 30 months after target discovery began.¹⁷ The integrated AI-driven workflow allowed to accelerate the development timeline, progressing from initial target identification to a preclinical candidate in just 18 months.¹⁸ One year later, the company announced that the drug had advanced to phase II.¹⁹ As explained in the previous section, using traditional methods for the same drug development process would have cost more than \$400 million and taken up to six years.²⁰ But with generative AI, Insilico declared to have achieved them at one-tenth the cost and reduced the timeline to two and a half years. *Rentosertib*, the official non-proprietary name adopted in 2025, is the first reported investigational drug in which both the biological target and the therapeutic compound were discovered using generative AI.²¹

In 2023, another generative AI drug company reported a breakthrough in antibody design using computer (*in silico*) methods.²² The company used generative AI to computationally design antibodies without starting from known natural binders (also known as “de novo”), as is usually done. In this wake, generative AI models are trained on large datasets of known molecules and their properties. From this data, they learn the basic principles of chemistry and biology to design entirely new molecules tailored to specific targets in the human body.²³ This promise of AI-driven antibody design could enable the targeting of diseases previously impossible to treat. Equally important, it would also speed up the discovery process by testing and optimising drug properties *in silico* rather than through slow lab experiments. *De novo* antibody design is technically challenging because of the enormous complexity of protein space and the need for atomic-level precision. Recent AI advances suggest such precision may become possible. Another example of this is AlphaFold 3, the most recent version of Google’s DeepMind AI engine, which can predict protein structures with remarkable accuracy. Determining protein structures and their interactions would have traditionally taken years of labour-intensive experimentation.²⁴ This advancement was recognised with the 2024 Nobel Prize in Chemistry to its creators.²⁵

¹⁷ InSilico Medicine, From Target discovery to phase 1 initiation in under 30 months: AI-discovered and designed drug enters the clinic, Available at: <https://www.nature.com/articles/d43747-022-00112-7> (June 2022).

¹⁸ Nvidia, Quicker Cures: How Insilico Medicine Uses Generative AI to accelerate Drug Discovery. Available at: <https://blogs.nvidia.com/blog/insilico-medicine-uses-generative-ai-to-accelerate-drug-discovery/> (27 June 2023)

¹⁹ Ibid.

²⁰ See, Section §1.

²¹ See: <https://www.news-medical.net/news/20250307/Insilico-Medicines-AI-driven-drug-Rentosertib-receives-official-generic-name.aspx> (7 May 2025). In June 2025, the company also announced to have advanced to Phase IIb: <https://insilico.com/news/tncrcuxsc1-insilico-announces-nature-medicine> (June 2025).

²² Shانهsazzadeh, Amir & Bachas, Sharrol & Kasun, George & Sutton, John & Steiger, Andrea & Shuai, Richard & Kohnert, Christa & Morehead, Alex & Brown, Amber & Chung, Chelsea & Luton, Breanna & Diaz, Nicolas & Mcpartlon, Matthew & Knight, Bailey & Radach, Macey & Bateman, Katherine & Spencer, David & Cejovic, Jovan & Kopeck-Belliveau, Gaelin & Meier, Joshua. (2023). Unlocking de novo antibody design with generative artificial intelligence. 10.1101/2023.01.08.523187. However, the company also faced some criticism that some touted “de novo” antibodies were actually optimized or redesigned versions of existing antibodies. See: <https://www.genengnews.com/topics/artificial-intelligence/scratch-that-de-novo-antibody-design-enters-the-ai-drug-discovery-toolbox/>.

²³ Drug Patent Watch, Generative AI Can Design Drugs, But Can it Own them?. Available at: <https://www.drugpatentwatch.com/blog/generative-ai-can-design-drugs-but-can-it-own-them/> (9 July 2025).

²⁴ Google, AlphaFold 3 predicts the structure and interactions of all of life’s molecules (08 May 2024). Available at < <https://blog.google/technology/ai/google-deepmind-isomorphic-alphafold-3-ai-model/> >. Last accessed: 16 December 2025. The AlphaFold 3 version was first introduced in an article. See: Abramson, J., Adler, J., Dunger, J. *et al.* Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature* **630**, 493–500 (2024). <https://doi.org/10.1038/s41586-024-07487-w>

²⁵ The creators of AlphaFold 2 have been awarded the 2024 Nobel Prize. See: The Royal Swedish Academy of Sciences, *Press Release: They cracked the code for proteins’ amazing structures*, <https://www.nobelprize.org/prizes/chemistry/2024/press-release/> (October 9, 2024)

As things stand, this does not come as a surprise that several pharmaceutical companies are forming partnerships with AI-focused firms.²⁶ In 2025, AI for drug discovery emerged as the leading segment with \$949 million in investment.²⁷ Around 69% of pharmaceutical companies are investing in AI for drug development.²⁸

2. Patents in the AI drug discovery process: which strategy?

In the pharma sector, patent protection is the cornerstone of the pharmaceutical business model.²⁹ These rights enable companies to recoup substantial investments in R&D while also providing incentives for continued innovation. Patents also balance innovation with accessibility by allowing generic drug production after the patent expires, making treatments more affordable. Additionally, patents foster collaboration and help navigate regulatory challenges, ensuring the pharmaceutical industry remains dynamic and innovative.³⁰ Pharmaceutical companies tend to file patent applications identifying promising drug candidates once drug discovery has concluded but before drug development begins. This means filing after pre-clinical testing has concluded but before clinical trials in humans have begun.³¹ The 20-year exclusivity granted by patent rights is thus central to forecasting the financial return on investment in developing a drug product. The reliance on patent protection is likely to influence every investment decision made by pharmaceutical companies, from funding new clinical trials to entering in collaborations with new companies and pursuing acquisitions.³²

With the increased use and development of AI tools for drug discovery, pharmaceutical companies are likely to create a wide range of technologies worth seeking patent protection. AI-driven drug discovery offers substantial patenting opportunities that may even exceed those of traditional methods.³³ This is because inventions in AI-driven drug discovery lie at the intersection of software and

²⁶ For instance, AI company BenevolentAI partnered with AstraZeneca in 2019. See: Benevolent AI and AstraZeneca Collaboration yields continued success as further novel target progressed into portfolio, (25 June 2024). Available at: <https://www.benevolent.com/news-and-media/press-releases-and-in-media/benevolentai-and-astrazeneca-collaboration-yields-continued-success-further-novel-target-progressed-portfolio/>; Eli Lilly has formed a multi target alliance with start up Atomwise to support preclinical drug discovery. See: Lilly and Atomwise partner to use AI for drug discovery. Available at: <https://www.pharmaceutical-technology.com/news/lilly-atomwise-ai-drug-discovery/> (June 2019).

²⁷ <https://tech.eu/2025/04/22/europes-healthtech-and-ai-startups-raise-139b-in-q1-as-global-investors> (April 2025).

²⁸ Midhat Tilawat, AI in Drug Development Statistics 2026: The \$60 Billion reality vs. Hype Analysis: <https://www.allaboutai.com/resources/ai-statistics/drug-development/> (1 January 2026)

²⁹ Hughes Rose, Why patents matter: understanding the importance of IP in the pharma industry, available at < <https://ipkitten.blogspot.com/2025/07/why-patents-matter-understanding.html> > (23 July 2025).

³⁰ <https://www.simsonpharma.com/blog-details/why-are-patents-important-to-drug-development> (9 September 2024). For a different view, see: <https://yalelawjournal.org/feature/does-pharma-need-patents> (questioning whether strong patent protection is essential for pharmaceutical innovation. The notes that that drug development relies on both compound knowledge and clinical trial data. While patents protect compounds, they play a limited role in incentivising early research, whereas clinical data drive most costs but are poorly protected by patents. The author therefore advocates for tailored regulatory exclusivity as a more effective way to support innovation, reduce inefficiencies, and improve access to medicines).

³¹ See: Christopher Garrison, Pharmaceutical patents and data exclusivity in an age of AI-driven drug discovery and development, *Medicines Law & Policy* (15 April 2025). Available at < <https://medicineslawandpolicy.org/2025/04/pharmaceutical-patents-and-data-exclusivity-in-an-age-of-ai-driven-drug-discovery-and-development/> >.

³² Hughes Rose, Why patents matter: understanding the importance of IP in the pharma industry, available at < <https://ipkitten.blogspot.com/2025/07/why-patents-matter-understanding.html> > (23 July 2025).

³³ From a technical perspective on AI-driven drug discovery opportunities, see: Kant, S., Deepika & Roy, S. Artificial intelligence in drug discovery and development: transforming challenges into opportunities. *Discov. Pharm. Sci.* **1**, 7 (2025). <https://doi.org/10.1007/s44395-025-00007-3>; Ferreira FJN, Carneiro AS. AI-Driven Drug Discovery: A Comprehensive Review. *ACS Omega*. 2025 Jun 6;10(23):23889-23903. doi: 10.1021/acsomega.5c00549. PMID: 40547666; PMCID: PMC12177741.

life-science technologies, including biotech. These industries rely heavily on patent protection for their inventions.³⁴

That said, within the arena of AI-driven drug discovery, patent protection may extend to several key elements of innovation. First and foremost, companies might be interested in protecting the resultant products developed through the AI-driven discovery activities. In this regard, companies may seek patent protection for pharmaceutical compounds identified through AI, including both small-molecule drugs and biologics, such as antibodies. Patent claims may also extend to therapeutic methods using these compounds, as well as diagnostic tools or manufacturing processes generated or optimised by AI systems.³⁵

Patent protection may be sought not only for the resulting products but also for the technologies used to create them, e.g. for the AI algorithms and model architectures used. For instance, companies seeking to build an AI drug-discovery platform may seek patent protection for the technology itself (i.e. the platform and the underlying technical methods).³⁶ Companies might also seek protection for the supporting hardware device and software that implement those algorithms. The methods and processes employed to perform drug discovery tasks might also be protected.³⁷

On the one hand, companies are likely to pursue patents for inventions across both software and biotech domains to build strong portfolios. On the other hand, existing patent frameworks may struggle to accommodate the distinctive characteristics of AI-driven innovation. In this sense, there is a body of literature that has addressed the challenges posed to patent law when attempting to patent algorithms, devices, and processes implemented in AI devices and tools.³⁸

Building on this literature, the remainder of this article will shift focus to one of these challenges, i.e., the sufficiency of disclosure requirement in the specific context of AI-driven drug discovery. While some scholars have addressed the disclosure requirements for AI-related inventions in general, their

³⁴ European Patent Office, 2024 Patent Index. Available at: < <https://www.epo.org/en/about-us/statistics/patent-index-2024/statistics-and-indicators/european-patent-applications/top-10-technical-fields> >. (3 February 2025).

³⁵ Hughes Rose, IP Strategy for AI-Assisted drug discovery. Available at: < <https://ipkitten.blogspot.com/2024/10/ip-strategy-for-ai-assisted-drug.html> > (31 October 2024); Chun, Matthew, Artificial Intelligence for Drug Discovery: A New Frontier for Patent Law (August 30, 2023). Journal of the Patent & Trademark Office Society (Forthcoming), Available at SSRN: <https://ssrn.com/abstract=4566014> or <http://dx.doi.org/10.2139/ssrn.4566014>

³⁶ Hughes Rose, IP Strategy for AI-Assisted drug discovery. Available at: < <https://ipkitten.blogspot.com/2024/10/ip-strategy-for-ai-assisted-drug.html> > (31 October 2024).

³⁷ Jayeoba, Ayodeji, Recalibrating Pharmaceutical Regulatory Exclusivities in the Age of AI (September 09, 2024). Available at SSRN: <https://ssrn.com/abstract=5126246> or <http://dx.doi.org/10.2139/ssrn.5126246>.

³⁸ See indicatively: Enrico Bonadio and Magali Contardi, Artificial intelligence, patents and health innovation". In *Intellectual Property Rights in the Post Pandemic World* (Eds), Cheltenham, UK: Edward Elgar Publishing 2023, (pp. 188-204); Contardi, Magali, Patentability of Diagnostic Methods: European and US Approach at a Comparison (november 01, 2023). (2023) 45 E.I.P.R., Issue 12, Available at SSRN: <https://ssrn.com/abstract=4738637> (on patentability of AI-devices for diagnostic). In that regard, at the outset, it should be noted that certain patent law challenges are not specific to drug discovery but are associated with the use of AI technologies in general. Among them, scholarly work has addressed issues of inventorship and patent eligibility for AI inventions. See indicatively: Martin Stierle, 'A De Lege Ferenda Perspectives on Artificial Intelligence Systems Designated as Inventors in the European Patent System' (2021) GRUR Int 115, 125-126 (pointing out also the specific difficulties if patent laws were to acknowledge AI inventorship); Noam Shemtov and Garry A Gabison, 'The inventive step requirement and the rise of AI machines' in Ryan Abbott (ed), *Research Handbook on Intellectual Property and Artificial Intelligence* (Elgar 2022); Gurgula, Olga, AI-Assisted Inventions in the Field of Drug Discovery: Readjusting the Inventive Step Analysis (August 29, 2020). International Journal of Social Science and Public Policy, Vol. 2, No. 8; August 2020, Available at SSRN: <https://ssrn.com/abstract=3683127>; Fabris, Daniele, From the PHOSITA to the MOSITA - Will 'Secondary Considerations' Save Pharmaceutical Patents From Artificial Intelligence? (February 9, 2020). 52 International Review of Intellectual Property and Competition Law 2020, Available at: SSRN: <https://ssrn.com/abstract=3623078> or <http://dx.doi.org/10.2139/ssrn.3623078> From The Phosita To The Mosita - Will "Secondary Considerations" Save Pharmaceutical Patents From Artificial Intelligence? IIC, 52; Abbott, R. (2018).

application in the pharmaceutical domain raises distinct concerns.³⁹ In particular, the use of AI in drug discovery has prompted arguments that existing patentability standards in biotechnology and pharmaceuticals remain too low.⁴⁰ According to this view, when standards are applied too leniently, patents might be granted for outputs routinely generated by AI.

Related concerns have been raised by Freinlich and Rai, who, in an empirical study conducted on granted drug compounds from over 100 AI-drug companies, identified a trend toward premature patenting.⁴¹ They observed that AI-driven drug companies increasingly file patent applications for compounds supported by limited experimental validation. Unlike traditional pharma, such patents are based on computational predictions rather than biological testing. On this basis, they argued that such early patenting may protect speculative molecules that are unlikely to be developed into viable therapies, with the risk of creating exclusionary rights that deter follow-on research by competitors.

Against this background, this article contributes to this ongoing scholarly discussion by re-examining the sufficiency disclosure for AI-driven drugs under European patent law. Its analysis is twofold. First, it clarifies how disclosure requirements are currently interpreted and applied to AI-driven drug inventions. Second, it assesses if the existing disclosure standards remain fit for purpose in light of increasingly data-driven and computational innovation. In this way, the article advances policy-oriented reflections on how European patent law can balance incentives for innovation with the need to prevent overly broad or speculative patent protection. Incidentally, it provides practical recommendations for practitioners drafting and prosecuting patent applications in AI-driven drug discovery.

3. *In silico* data and the disclosure conundrum in AI-driven drug discovery

In European patent law, to be granted patent protection, an invention must be novel, involve an inventive step, and have an industrial application.⁴² Moreover, Article 83 European Patent Convention (EPC) stipulates that the application shall disclose the invention in a manner sufficiently clear and complete for it to be carried out by a person skilled in the art. This latter requirement is known as sufficiency of disclosure.

Disclosure is at the heart of the “patent bargain”. Under this *quid pro quo* agreement, a patent owner receives a limited term of exclusivity for the invention in exchange for publicly disclosing how to make and use it after the expiration of the patent. Unlike novelty or inventive step, disclosure deficiencies are particularly problematic because they cannot normally be remedied after filing. The content of the application as filed largely determines the outcome of patent protection.⁴³ Failure to meet the disclosure requirement means the patent bargain is violated. As a result, a patent application may be rejected, while a granted patent may be revoked or held invalid.⁴⁴

³⁹ Mateo Aboy, Aparajita Lath, Timo Minssen, Kathleen Liddell, The sufficiency of disclosure of AI inventions, *Journal of Intellectual Property Law & Practice*, Volume 19, Issue 11, November 2024, Pages 834–840, <https://doi.org/10.1093/jiplp/jpac063>

⁴⁰ Gurgula, Olga, AI-Assisted Inventions in the Field of Drug Discovery: Readjusting the Inventive Step Analysis (August 29, 2020). *International Journal of Social Science and Public Policy*, Vol. 2, No. 8; August 2020, Available at SSRN: <https://ssrn.com/abstract=3683127>;

⁴¹ Janet Freinlich, Arti K. Rai, What patents on AI-derived drugs reveal. *Science* **388**, 924–926 (2025). DOI: [10.1126/science.adw1972](https://doi.org/10.1126/science.adw1972)

⁴² Articles 52, 54, 56 and 57. Convention on the Grant of European Patents (European Patent Convention) (adopted 5 October 1973, entered into force 7 October 1977) 1065 UNTS 199 (EPC).

⁴³ EPO Case Law of the Boards of Appeal 2025, Part III, C.2 and 7. Available at: https://www.epo.org/en/legal/case-law/2025/clr_ii_c_2.html It shall be noted that the use of post-filed documents is controversial. See. Part III, C, 7.

⁴⁴ Di Giovine, Paolo, Patentability of AI-based Inventions in the Pharmaceutical Field Under the European Patent Law *European Health & Pharmaceutical Law Review* Volume 8, Issue 4 (2025) pp. 245 – 250 DOI: <https://doi.org/10.21552/ehpl/2025/4/9>.

The disclosure requirement in the biotech and pharma fields assumes particular relevance. In this area, inventions covering drug compounds are often defined by their biological activity or therapeutic effect, rather than by easily observable structural features alone. Thus, applicants are expected to demonstrate that the drug candidate for which patent protection is sought has the therapeutic effect that it is claimed in the application.⁴⁵ However, as Section II discussed, in the pharmaceutical field, patent applications are often filed before full clinical trials are initiated. Consequently, the evidence available at the filing date to render the technical effects of the invention robust is often limited. In this context, the key question is how much needs to be disclosed and how much experimental data is enough to demonstrate the claimed effect of the drug compounds.

Under the European Patent Office (EPO) practice, the patent must enable the skilled person to carry out the invention across the whole scope claimed. This assessment is based on common general knowledge at the priority date. The invention must be workable without “undue burden”.⁴⁶ In practice, the bar for sufficiency is relatively low. In principle, it is not necessary to submit any clinical trial data. However, applicants must submit credible technical evidence that the compound or biological agent plausibly solves the technical problem it purports to address.⁴⁷ Guidelines for Examination state that disclosing a single example may suffice, provided that the claimed therapeutic effect is unambiguously reflected.⁴⁸ For instance, in antibody claims, the EPO requires that the patent disclose at least one clear and reproducible method for obtaining antibodies within the scope of the claims.⁴⁹ Applicants would, hence, typically provide laboratory data showing that the drug binds its target and produces the claimed therapeutic effect. Similarly, chemical-molecule product claims require disclosure of how to make the product (i.e. its synthesis or preparation method), and a detailed description thereof, the structure, composition, and any unique properties. By contrast, sufficiency is not met if the skilled person must undertake an undue trial and error research programme to reproduce the results of the invention.⁵⁰

AI-driven drugs alter this landscape. As section 1 showed, companies increasingly rely on computational models of biological phenomena rather than on data collected from “real-world” experiments, such as laboratory assays, animal studies or clinical trials. Similarly, the emergence of highly accurate *in silico* prediction tools, such as AlphaFold 3, rapidly generates large numbers of candidate molecules or predictions. They allow researchers to test multiple hypotheses rapidly and at scale while exercising precise control over experimental variables across virtually unlimited computational runs.⁵¹

⁴⁵ This is also known as plausibility. There is no statutory basis in the EPC yet the term appears in numerous Board of Appeal decisions under sufficiency assessment (Art. 83 EPC) or inventive step (art. 56 EPC). In relation to sufficiency of disclosure, this concept generally concerns the idea that a purported effect of the claimed invention, e.g., a treatment of a particular disease, must have been credible to the skilled person at the time of filing of the application based on the disclosure in the application as filed. The Enlarged Board of Appeal attempt to provide some guidance on this requirement in G2/2021. See: Enlarged Boards of Appeal of the EPO (EBoA), G 2/21. See also: Yelena Morozova, Craig Slater and others, Patent plausibility Uncertainty Persists, EPO petition Shows, Finnegan (18 March 2024), Law360, Available at: <https://www.finnegan.com/en/insights/articles/patent-plausibility-uncertainty-persists-epo-petition-shows.html> . See also: Rose Hughes, Plausibility demystified – a review of EPO case law before G 2/21, (24 February 2023), IPKat. Available at: <https://ipkitten.blogspot.com/2023/02/plausibility-demystified-review-of-epo.html> .

⁴⁶ EPO Guidelines 2025, at F-III-1.

⁴⁷ Ibid, (fn 43).

⁴⁸ EPO Guidelines 2025, at F-III, 1; EPO Boards of Appeal (BoA), T801/06.

⁴⁹ EPO Guidelines 2025, at F-IV, 4.11 and G-III-6.1. See also:

⁵⁰ EPO Boards of Appeal (BoA), T 38/11, Reasons 2.6.

⁵¹ In the fields of antibody, *in silico* modelling significantly reduces the experimental burden previously associated with reproducing the full scope of functionally defined antibody claims. As Bohrer et al. explain, traditionally, broad antibody claims have struggled to meet sufficiency requirements because the skilled person would need to generate and experimentally screen a vast number of candidates to identify those that bind the claimed antigen with the desired properties. Recent advances in protein structure prediction, exemplified by AlphaFold 3, materially alter this assessment. Once an antibody targeting a particular antigen has been shown to have therapeutic potential through laboratory experiments, AlphaFold 3 can model the three-dimensional interaction between the antibody and its antigen. See: Bohrer, Robert A. and Bargmann, Brendan,

There is, therefore, growing interest in using such computationally generated data to support patent applications. However, such use raises the question of whether computational or *in silico* evidence alone can establish the sufficiency and plausibility of a claimed technical effect. The question is not rhetorical. If the disclosure standard is applied too leniently, patents will be granted for outputs that are insufficiently characterised or experimentally validated.⁵²

At the EPO, there is no agreed standard for the use of *in silico* data to support the sufficiency of disclosure. Conversely, its use has been expressly accepted to demonstrate the industrial applicability, on the ground that it can “allow plausible conclusions to be made regarding the function of a product before it is actually tested.”⁵³ It has also been accepted to support inventive step.⁵⁴ As a result, the case law addressing whether such data alone can support the plausibility of a claimed therapeutic effect remains underdeveloped.⁵⁵ Some commentators have therefore cautioned that AI-drug discovery companies must take particular care not to file patent applications too early, when only computational data is available.⁵⁶ This is because the final drug product may therefore differ materially from the molecule initially identified *in silico*. An early filing risks failing to cover the eventual clinical lead and, in the worst scenario, becoming citable prior art against later applications directed to the optimised compound.⁵⁷ Others have proposed that *in silico* data should not stand alone, but should be supported by wet-lab experimental evidence. According to this view, this would be consistent with the long-standing practice of relying on empirical data to demonstrate technical effects in pharmaceutical patent applications.⁵⁸

A related issue for patent applicants is whether the use of AI-generated data to support a patent claim requires disclosure of the AI model used.⁵⁹ Some have contended that the reliability of *in silico* data

AlphaFold 3, AI, Antibody Patents, the Future of Broad Pharmaceutical Patent Claims, and Drug Development (June 26, 2025). AIPLA Quarterly Journal, Volume 53, No. 2. Pp. 247-276, Available at SSRN: <https://ssrn.com/abstract=4983123> or <http://dx.doi.org/10.2139/ssrn.4983123>

⁵² A related challenge is how drug regulatory agencies will assess candidate drugs using AI, especially in terms of the reliability of *in silico* modelling data and the extent to which such data could eventually replace conventional preclinical studies. See: Christopher Garrison, Pharmaceutical patents and data exclusivity in an age of AI-driven drug discovery and development, *Medicines Law & Policy* (15 April 2025). Available at < <https://medicineslawandpolicy.org/2025/04/pharmaceutical-patents-and-data-exclusivity-in-an-age-of-ai-driven-drug-discovery-and-development/>>. In the EU, a guideline development is already underway, building on the EMA AI Reflection paper published in 2024 See: European Medicine Agency, Reflection paper on the use of AI in the medicinal product lifecycle (2024), Available at: https://www.ema.europa.eu/en/documents/scientific-guideline/reflection-paper-use-artificial-intelligence-ai-medicinal-product-lifecycle_en.pdf. In January 2026, EMA and the U.S. Food and Drug Administration (FDA) have jointly identified ten principles for good artificial intelligence (AI) practice in the medicines lifecycle. See: <https://www.ema.europa.eu/en/news/ema-fda-set-common-principles-ai-medicine-development-0>, (14 January 2026).

⁵³ BoA, T 835/21, reason §22

⁵⁴ In decision T 2517/19, the Board of Appeal held that experimental results obtained for antibodies could be credibly extrapolated to corresponding antibody–drug conjugates, relying on *in silico* analysis to support inventive step.

⁵⁵ 17 is mentioning that with its ruling on November 25, 2025 (UPC_CoA_529/2024), the UPC Court of Appeal confirmed that sufficiency does not require the patent to experimentally validate every conceivable embodiment falling within a functionally defined claim. What matters is whether the skilled person, using the disclosure and common general knowledge at the priority date, can reliably obtain antibodies with the claimed functional properties with a reasonable amount of trial and error and without undue burden. This suggests that sufficiency would be met regardless of whether that enablement is achieved through wet-lab experiments, computational modelling, or a combination of both.

⁵⁶ Hughes Rose, IP Strategy for AI-Assisted drug discovery. Available at:< <https://ipkitten.blogspot.com/2024/10/ip-strategy-for-ai-assisted-drug.html> > (31 October 2024).

⁵⁷ Moreover, although not related to AI, as illustrated in decision T 0709/23 of 16 June 2025, where post-published data is accepted, it can undermine sufficiency if it contradicts the technical teaching of the application as filed.

⁵⁸ Laura Fe, IP Considerations of Generative AI in Drug Development and materials Discovery (8 October 2024). Available at: <https://www.murgitroyd.com/insights/patents/applications-of-generative-ai-in-drugs-development-and-materials-discovery-ip-considerations>; Ella Green, Gary Small and ben Husband, Patenting AI: AI and Drug Discovery (16 June 2022). Available at: <https://www.carpmaels.com/patenting-ai-artificial-intelligence-and-drug-discovery/>

⁵⁹ The author has discussed this issue as speaker during the 2025 AIPPI world Congress in the Panel ‘Artificial Creativity or Intellectual reality: Use of Generative AI in Pharma and Biotech and its impact on the patenting process’. The discussion has been capture by Marisa Woutersen in the article to disclose or not: Pharma patents face new AI reality, *Life Sciences IP* in

is difficult to assess when the details of the model are not provided.⁶⁰ However, this matter is sensitive, as many algorithms are proprietary, and companies are interested in keeping their research processes confidential. Requiring disclosure of such algorithms could risk eroding trade secrets. It might also render inventions obvious if it can be shown that the AI would inevitably produce the same result when given a particular problem.⁶¹ On the other hand, when AI leads to a novel drug or a new therapeutic use of a known drug, applicants may choose to claim only the drug or its new use. The model used to identify and select them may instead be kept as a trade secret.⁶²

At the outset, there is no specific provision in the EPC and EPO Guidelines. The answer to the above question should be answered following the established principles laid down in the EPC. As mentioned at the beginning of this section, the disclosure requirement under Article 83 EPC focuses on enabling the skilled person to carry out the invention. It does not require reconstructing the research pathway or the inventive process. Therefore, if the claimed invention is an AI output, such as a compound obtained with AI, the disclosure requirement for that AI output should be the same as with any other invention. Consequently, if a molecule discovered via AI could also have been obtained using conventional methods, the AI itself is largely irrelevant to sufficiency. Accordingly, sufficiency should be assessed by reference to the claimed product, not the method or technology by which it was discovered.

Conversely, a disclosure obligation should arise only where knowledge of the AI method is necessary for enablement, that is, obtaining the invention.⁶³ In such circumstances, the disclosure obligation may extend to the AI model itself or the data used. This is because the skilled person would otherwise be unable to reproduce the invention without understanding the specific characteristics of the AI system. This would be consistent with the Guidelines for Examination, as updated following decision T0161/18.⁶⁴ According to the Guidelines, while mere assertions of technical effect are insufficient, comprehensive proof is not required. However, if a technical effect depends on particular characteristics of a machine learning model or its training data, those characteristics must be disclosed. An exception to

Review (16 September 2025). Available at: <https://www.lifesciencesipreview.com/asia/to-disclose-or-not-pharma-patents-face-new-ai-reality>

⁶⁰ Aleksandra Kinebas, In silico data at the EPO: Future strategies for biotech patents, (November 2025). Available at: <https://www.kilburnstrode.com/knowledge/european-ip/in-silico-data-epo-futureproof-strategies-biotech>. See also: Jayeoba, Ayodeji, Recalibrating Pharmaceutical Regulatory Exclusivities in the Age of AI (September 09, 2024). Available at SSRN: <https://ssrn.com/abstract=5126246> or <http://dx.doi.org/10.2139/ssrn.5126246> (Advocating that a balanced disclosure standard for AI-assisted pharmaceutical inventions can serve as a catalyst for generic and biosimilar competition, and stressing that comprehensive, yet reasonable, requirements for disclosing the AI systems and processes used in drug discovery can help manufacturers navigate the complexities of replicating patented drugs without undue experimentation).

⁶¹ Gurgula, Olga, AI-Assisted Inventions in the Field of Drug Discovery: Readjusting the Inventive Step Analysis (August 29, 2020). International Journal of Social Science and Public Policy, Vol. 2, No. 8; August 2020, Available at SSRN: <https://ssrn.com/abstract=3683127>.

⁶² Di Giovine, Paolo, Patentability of AI-based Inventions in the Pharmaceutical Field Under the European Patent Law European Health & Pharmaceutical Law Review Volume 8, Issue 4 (2025) pp. 245 – 250 DOI: <https://doi.org/10.21552/ehpl/2025/4/9>.

⁶³ Ibid. p. 4. Another example in which disclosure of the AI becomes necessary is where the AI technology itself forms part of the claimed invention. This may arise where the outputs of the AI process are not patentable as such, for example the identification of a new molecular pathway or a protein–protein interaction. In such situations, the only potentially patentable subject matter lies in the AI-driven process itself. To meet the sufficiency of disclosure requirement, the patent application must then describe the AI method in sufficient technical detail to allow the skilled person to reproduce it.

⁶⁴ Equivalent aortic pressure/ARC Seibersdorf) of 12 May 2020. For an overview of this decision, See: Enrico Bonadio and Magali Contardi, Artificial intelligence, patents and health innovation". In *Intellectual Property Rights in the Post Pandemic World* (Eds), Cheltenham, UK: Edward Elgar Publishing, (pp.188-204).

the disclosure would be that they can be derived by a skilled person without undue burden.⁶⁵ The EPO does not generally require disclosure of the specific training dataset itself.⁶⁶

Against this background, interpreting Article 83 EPC so as to introduce a general duty to disclose the use of AI where the AI process is not directly claimed would be problematic. It would risk conflating patent law with broader regulatory goals such as transparency or explainability.⁶⁷ It would also impose an additional criterion that is not supported by European patent law or international agreements. Article 27 of the TRIPS Agreement bases patentability on the invention itself, irrespective of how it was developed. As a result, companies could be prompted to rely on trade secrets instead of patents.⁶⁸

4. Conclusion

The use of AI in drug-discovery to transform the landscape by accelerating target identification, optimising lead compounds, and even designing novel molecules or antibodies entirely *in silico*. This shift, however, raises important questions for European patent law, in particular for the sufficiency of disclosure requirement stipulated under Article 83 EPC. In pharmaceuticals, this requirement has traditionally required empirical evidence demonstrating a plausible therapeutic effect. AI-generated inventions challenge this model because they often rely on computational predictions rather than wet-lab data at the time of filing. The EPO accepts *in silico* evidence for industrial applicability and inventive step. However, it has not yet established a consistent standard for sufficiency of disclosure based solely on computational data.

In a landscape where drug development remains costly, slow, and uncertain, AI offers unprecedented opportunities to accelerate and expand the search for new therapeutics. As AI systems generate increasingly complex and numerous candidate molecules, the EPO will need to clarify how computational evidence fits within the sufficiency and plausibility framework. The patent system must continue to reward genuine technical contributions without granting protection for inadequately supported predictions. At the same time, it must avoid disclosure obligations that would stifle innovation or undermine the incentives driving AI-driven discovery. Maintaining this equilibrium will be critical for ensuring that the patent system continues to function as an engine of scientific and medical progress.

⁶⁵ EPO Guidelines, Part G-II, paragraph 3.3.1.

⁶⁶ Ibid. See also: Mateo Aboy, Aparajita Lath, Timo Minssen, Kathleen Liddell, The sufficiency of disclosure of AI inventions, *Journal of Intellectual Property Law & Practice*, Volume 19, Issue 11, November 2024, Pages 834–840, <https://doi.org/10.1093/jiplp/jpae063>

⁶⁷ Such as the transparency requirements introduced with the European Union, *Regulation (EU) 2024/1234 of the European Parliament and of the Council on Artificial Intelligence (AI Act)* [2024] OJ L 150/1 (AI Act).

⁶⁸ Tabrez Y Ebrahim, ‘Artificial Intelligence Inventions and Patent Disclosure’ (2020) 125 *Pennsylvania State Law Review* 147, 183.