International Journal of Technology and Applied Science (IJTAS)

E-ISSN: 2230-9004 ● Website: www.ijtas.com ● Email: editor@ijtas.com

In Silico Drug Repurposing Vs. Anti-Evergreening: Navigating Section 3(D) Of the Indian Patents Act in Light of Us and Chinese Patent Approaches

Honey Passi[1], Dr. Pushpanjali Sood[2]

[1]Scholar, Master of Laws, University Institute of Legal Studies, Chandigarh University, Mohali, Punjab, India

[2]Associate Professor, University Institute of Legal Studies, Chandigarh University, Mohali, Punjab, India

Abstract:

In silico drug repurposing involves computational methods such as molecular docking, network pharmacology, machine learning and structure-based prediction to discover new therapeutic uses for already existing drugs. These approaches can speed up drug discovery and lower development costs, but they do have some problems from the point of view of pharmaceutical patentability and how to avoid evergreening. This paper then explores these issues in the light of Section 3(d) of the Patents Act, 1970, by comparing the effectiveness-based exclusion under the Patents Act with the general patentability criteria in the United States and patentability of pharmaceutical-use claims in China. The doctrinal and comparative approach is applied in examining relevant legislation, court rulings, and patent examination documents, to distinguish the practice of therapeutic innovation from an over-ambitious extension of existing patent monopolies by "tinkering" with existing products. It states that computer-discovered items are deserving of neither automatic acceptance of patentability nor automatic exclusion from patentability. Rather, it is the substantive novelty, inventive step, disclosure and evidence which should establish patentability, and not just because of the use of AI. The paper also suggests that while aiming to retain the public health goals of Section 3(d), India should make sure that such goals are applied in the spirit of the patent law, namely on the basis of novel therapeutic uses, including those with respect to a new method of treatment, and not with respect to a new chemical entity. The comparative analysis finally suggests a claim-sensitive approach that strikes a balance between pharmaceutical innovation and access to medicines on the one hand, and patent integrity on the other, while maintaining the purpose of anti-evergreening protection.

Keywords: In silico drug repurposing, section 3(d), pharmaceutical patents, evergreening, artificial intelligence, India; United States, China.

Introduction:

The study of drug repurposing—also referred to as drug repositioning-is the process of looking for a new therapeutic application for a drug with known pharmacological characteristics, safety profile or clinical performance. Computational techniques can be used to analyze vast sets of chemical and biological information, to predict drug–target interactions, to model molecular binding, and discover disease pathways. These approaches can provide ideas for new drugs sooner than de novo drug discovery. However, a computational prediction is not a clinically effective treatment and a prediction alone is not necessarily a patentable invention. The question before the law is whether the application contributes and is not obvious in the technical sense, and whether it is adequately disclosed and supported by evidence.

This is a particular concern in India. Under section 3(d) of the Patents Act, 1970 the mere discovery of a new form of a known substance, which does not show an improved known efficacy, and the mere discovery of a new property or new use of a known substance, are excluded. Its explanation identifies specified derivatives—such as salts, esters, ethers, polymorphs, metabolites, pure forms, particle sizes, isomers, mixtures and other derivatives—as the same substance unless they differ significantly in properties with regard to efficacy. The purpose of the provision is to prevent patents for "incremental change" that are not worth granting an additional monopoly.

But, not all repurposing is equal to evergreen. Although the active substance is a relatively old one, the new indication could provide significant clinical advantages. On the other hand, a claim which is created by an algorithm would be speculative or obvious or not sufficiently disclosed. The big question is whether there is enough innovation in evidence to justify the extension of exclusivity without any comparable innovation. This paper proposes that there is a difference between (i) a new form of a known product, (ii) a new use of a known product, (iii) a new therapeutic use of a known product with supporting technical advantages, and (iv) a computational tool or workflow that, when applied to a known product, results in a patentable technical improvement.

Research Questions, Methods and Scope

The paper focuses on four questions: When in silico methods find a new use for an "old" drug, how should section 3(d) apply? Secondly, what is the difference between India and the patent regime in the United States and China in the context of pharmaceuticals? Finally, what proof would be needed to prove that it is a genuine reuse rather than evergreen? Lastly, how to implement changes that maintain access to medicines while not dissuading valuable computational studies?

The method adopted is doctrinal and comparative. It focuses on the statutory text, the leading cases and the official guidance to the exams, and secondary scholarship is utilized to identify practical concerns. The comparison is not an assertion that the three systems are one and the same or that any one system offers a comprehensive model for India. Patentability depends upon the claim and examination practice may vary. The paper concentrates on patent law and not regulatory approval, data exclusivity or reimbursement-although these can also shape incentives.

Scope of Scientific Promise and Patent Questions for In Silico Drug Repurposing

Molecular docking, virtual screening, molecular dynamics, machine-learning prediction, knowledge graphs, gene-expression analysis and network-based drug–disease relationship identification are all components of in silico repurposing. These techniques can be used to suggest potential candidates for laboratory testing, although the reliability of such techniques is dependent on the quality and

representativeness of training data, the assumptions made when using the technique and whether the technique has been experimentally validated in the context of this biological problem. The prediction of an interaction does not necessarily mean that it is safe and effective in humans.

The possible implications of the patent would be determined by the claims. A patent claim to a computational model or new data-processing pipeline might trigger patent-eligible subject matter and technical contribution/disclosure issues. A new chemical entity could be evaluated according to old product-patent criteria. A claim to an approved drug for a new disease can be made as a therapeutic use claim or (in some jurisdictions) a method-of-treatment claim. A claim to a new formulation, dosage regime, salt or polymorph may involve rules against secondary patents or "evergreening." These should never be combined into a single category.

Novelty and inventive step are not automatically given by the use of AI or computational prediction. Where the prediction was made through sophisticated software, but the new indication was apparent to an expert in the field based on existing literature, mechanism of action, or routine screening, the claim may not be accepted. Similarly, a computational indication that is identified could be inventive if it finds a non-obvious biological relationship and it is accompanied by reproducible experimental evidence. The claimed result and contribution over prior art, rather than the computational origin, should be considered in patent law.

India: Section 3(d), Therapeutic Efficacy and the Evergreening Concern

Section 3(d) of the Patents Act, 1970, should be interpreted in the light of the general requirements of invention, novelty and inventive step. It does not provide a full guideline on patentability of pharmaceutical products. Section 2(1)(j) defines an invention and section 2(1)(ja) requires that the invention involves technical advance over existing knowledge or economic significance or both and that it is not obvious to a person skilled in the art. Section 3(i) excludes separately methods of medical treatment of humans or animals. As such, a repurposing claim should be reviewed both as to language and substance; section 3(i) may be a concern for a method-of-treatment claim, while other issues may be raised for a claim directed to a substance or a claim properly framed as a pharmaceutical product.

The top case is Novartis AG vs. Union of India. The Supreme Court ruled against the claim of beta-crystalline form of imatinib mesylate as it failed to meet the requirement of improved known efficacy under section 3(d). In its pharmaceutical context, the Court took efficacy to mean therapeutic efficacy, and stressed that the applicant had failed to show that they had improved it. The court's judgment was not that all incremental innovations in the field of pharmaceuticals were not patents worthy; they required the threshold to be fulfilled by the evidence.

Novartis is significant but shouldn't be over-extended. It was not a simple calculation discovery of a new indication; it was a new form of a known substance. The language of 3(d) explicitly states that only the discovery of a new property or new use of a known substance would be excluded from 3(d) and no applicant would be able to exclude the invention simply by naming it "AI Enabled". Meanwhile, the efficacy test of the statutory explanation for derivatives shouldn't be automatically translated into a strict requirement that every new indication must demonstrate a percentage gain in the efficacy of the molecule for its previous indication. A novel indication is evaluated on its own clinical merit and the issue is not whether the indication is asserted, but whether the claim is a legally recognizable invention supported by an adequate level of scientific information and clinical trial data under the Act. This is vital.

Applications that claim a new disease for a known drug on the basis of a model output can be denied for the lack of credible disclosure, inventive step or proof of a real and enabled use. Section 3(d)'s requirement to show "enhanced efficacy" is directly engaged if the applicant relies on the same old indication and claims a new polymorph or formulation. Where a truly novel therapeutic indication is supported by substantial mechanistic, preclinical and clinical evidence, the examiner should evaluate on an independent basis whether section 3(d) precludes the claim, whether the claim form falls under section 3(i), and whether there is novelty and inventive step when considering the claim as a whole.

There are also obvious evidentiary concerns that arise from the provision. The above computational score is not evidence of therapeutic efficacy. But requiring such full clinical-trial data at the patent filing phase in each case would render the patent system ineffective for early stage research, but would allow large monopolies to be granted over potential treatments based on speculation. The threshold should be in line with the scope of the claim and the technical arguments set forth in the specification. The applicant is required to reveal the model and the relevant parameters to the extent relevant, to provide a biological rationale, and to provide sufficient data to make the claimed invention believable, or readily repeatable.

United States: General Patentability Rules and Therapeutic-Use Claims

There is no equivalent of section 3(d) in the United States. The three primary elements for patentability are found in the statutory language of 35 U.S.C. §§ 101, 102, 103 and 112: subject matter eligibility, novelty, non-obviousness, and written description/enablement. A new use of a known drug is acceptable as a method of treatment, as long as the claim meets the criteria and cannot be just a discovery or abstraction. Rather than a special test of the “pharmaceutical efficacy” of new versions of existing substances, the US approach provides a more general filter.

It does not imply that a new use automatically will be granted a patent. The USPTO's examination guidance acknowledges that a property of a known composition that is found to have a novel property does not render the known composition novel. A claim should identify an invention that is not obvious and covers a new invention. While the jurisprudence of obviousness is not specifically concerned with repurposing, the overall rule is that the claim is evaluated against the perspective of a skilled person looking to the prior art. Further, the specification should allow the scope to be fulfilled; if you claim an entire disease class based on a narrow computational prediction, it may be at risk.

A significant difference is that India's section 3(i) explicitly prohibits method-of-treatment claims, whereas the U.S. allows method-of-treatment claims. This may provide an opportunity to repurpose innovators with a novel format of the claimed molecule but without the molecule itself being novel. The enforceability and scope of such claims, however, are dependent upon the infringement doctrines, the claim language and the evidence that the claim is not obvious. Furthermore, the patentability of claims to algorithms or natural correlations does not change when the invention is made up of a computational method, as long as it is implemented using computers.

The US framework is applicable to repurposing when a particular new treatment approach is novel, non-obvious and enabled. The drawback is it does not have India's specific anti-evergreening clause for specified derivatives. While the general rules of novelty and non-obviousness may deny weak secondary claims, they are not necessarily going to solve the policy problem of providing a new term of monopoly for a trivial pharmaceutical change without any real therapeutic benefit. The section 3(d) of India can thus be interpreted not as alternative to the standard approach of patentability test, but rather as an additional tier of filtering.

China: Patentability, Medical-Use Claims and Technical Contribution

The Chinese Patent Law also demands novelty, inventiveness and practical applicability. There is an exception in Article 25 that does not permit methods for diagnosis or treatment of disease to be patented. In reality the pharmaceutical-use inventions have been handled by claim formats which aim to protect a method for making a medicament for a particular therapeutic purpose, and not merely to treat a patient. The availability and drafting of such claims will be determined by the applicable Patent Examination Guidelines, and the nature of the disclosure.

China does not have the same "section 3(d)" language for derivatives as India, but rather gives them a specific language of enhanced-therapeutic-efficacy. Rather, the assessment process usually focuses on the general patentability requirements and/or the examination of pharmaceutical claims such as novelty, technical effect, and the ability to tell the invention from the specification. The Patent Examination Guidelines of the China National Intellectual Property Administration (CNIPA), which were amended and came into effect in 2024, place great importance on disclosure and the provision of supporting experimental data in connection with relevant pharmaceutical contexts. It is especially relevant to the field of computational repurposing: An algorithmic prediction can lead to a research direction, but the application should still allow for the claimed medical use and should support the technical effect claimed. The comparison should be expressed clearly. Now that there is no equivalent of section 3(d) in China, it means that not all secondary pharmaceutical claims are patentable in China. Substantial barriers still exist, such as novelty, inventive step, sufficiency of disclosure and claim support. Nor does the same conduct receive the same scope of protection if it is a pharmaceutical-use claim in China, the United States and India. The determination of legal outcome can depend on exactly what claim category and examination practice can be found in the local jurisdiction.

The Chinese experience indicates that a strict examination of the disclosure and technical effect could be helpful in identifying speculative repurposing claims without using the India's exact wording. The public-health problem with a minor modification of a well-known drug can still not be adequately conveyed by disclosure. The verdict of 'distinct efficacy' filter is a conscious policy decision in India, which comparative law can help to shape up, but not wipe away the intention of law-making.

Comparative Analysis

The fundamental principle of the three systems is that a patent should be awarded for an invention, rather than a research idea. Both ask if the claim is novel and non-obvious, and both require specification communication. The main difference comes in the approach to novel applications, treatment procedures and secondary pharmaceutical modifications.

Table 1: Comparison with regards to Patent in three countries

Issue	India	United States	China
New therapeutic use	Section 3(d) expressly refers to a mere new use; section 3(i) excludes methods of treatment. Claim form	Method-of-treatment claims may be available if §§ 101–103 and 112 are satisfied.	Medical treatment methods excluded; pharmaceutical use claims may use accepted medicament-manufacture formats.

	and evidence are decisive.		
New form / derivative	Section 3(d) may require enhanced known efficacy for listed derivatives.	No direct section 3(d) equivalent; general novelty, non obviousness and disclosure apply.	General patentability and disclosure rules apply; no identical statutory efficacy filter.
Computational prediction	AI use alone does not prove invention; credible disclosure and legal eligibility are needed.	Algorithmic claims face eligibility and enablement requirements; treatment claims assessed normally.	Technical contribution, novelty, inventiveness and disclosure are important; a prediction alone is insufficient.
Policy emphasis	Express anti evergreening safeguard alongside ordinary patentability rules.	General patentability framework and potential method claims.	General patentability framework with specific examination guidance for pharmaceutical disclosure.

The comparison shows that there is no certain trade-off between innovation and access as competing objectives. A narrow patent can stop generic competition and a weak patent can cause a drop in investment in proving new uses of old drugs. In diseases where there is little commercial market, repurposing could be particularly useful, as the pharmacological information already available to the disease may help to mitigate some of the risks of research. However, the ability to have such a socially valuable research technique does not warrant a monopoly over all the predictions made by it.

Core Tension: Repurposing or Evergreening?

Evergreening refers to the practice of trying to prolong the commercial exclusivity of a product by obtaining subsequent patents for product changes, formulations, dosage forms and combinations, as well as new indications. Not all secondary patents are abuses. A new formulation that offers a significant increase in stability, adherence or safety could yield actual benefits. A new indication could also present a treatment choice for a disease without one. The difference is, however, not only between old and new molecules but it is between a claim that meets the requirements of the patent statute and one that is broader or has an evidentiary basis that is greater than what the applicant has actually invented.

This is exacerbated by in silico tools which can produce a large number of candidate associations at low marginal cost. As long as each association was able to get a wide patent without validating it, patent thickets would build up around current medicines and slow down independent research. However, if any potential use that is discovered by computational means were just considered a discovery, there might be valuable and non-obvious uses that are not incentivized. A principled system should be based on a clear claim, a credible technical justification, disclosure of the material methods and data, and evidence that is proportionate to the extent of the therapeutic claim.

The evidentiary question must be posed. The application should have enough information at the time of its filing to render the claimed invention creditable, reproducible and not depend on final assertions that efficacy is to be expected based on a model. As examination is carried out, the examiner should check the claim for novelty and closely determine if the specification covers the scope of the claim. Section 3(d)'s statutory requirement should be followed in cases of a new form of an existing substance, as interpreted by Novartis. If the claim relates to a new indication, the examiner should write a statement to explain why or why not the exclusion would apply, and to the specific claim.

Proposed Reforms For India

In the first place, the Indian Patent Office should provide instructions which are claim sensitive to the readers, addressing the interaction of section 3(d) and in silico repurposing. The guidance needs to separate out a new modification of an existing substance and a new indication, new method of treatment, new pharmaceutical formulation or computational invention. This would make it more predictable, without altering the wording of the statute.

Secondly, the material computational method should be disclosed in a manner which allows the skilled person to understand and perform the claimed contribution. The relevance disclosure can vary depending on the invention and can include data provenance and selection criteria, model architecture or essential parameters, validation protocol, limitations and experimental confirmation. This does not mean that there is a automatic obligation to share all source code lines or trade secrets – the law is that each line of code and trade secret is subject to the statutory "sufficiency" requirement. If claims are opaque, without an explanation of the output they produce, then they should not be broadly protected.

Thirdly, evidence must be relevant and claim-specific. Patent law should not always mandate completed human trials in all applications, as clinical development can be time consuming and could be regulated separately. The more robust and extensive the therapeutic claim, however, the more critical it is that the application has a plausible scientific basis for the claimed effect. Computational evidence can help support a hypothesis, but should not be considered as definitive evidence of clinical effectiveness.

Fourthly, the ordinary novelty and inventive-step analysis needs to be applied robustly by examiners. If there already exists a prior art disclosure of the therapeutic relationship or it would have been obvious to the person of skill in the art, then a new disease label upon the known molecule should not render that prior art inoperative. However, a new and promising therapeutic effect, if it occurs, should be evaluated individually. It is preferable for the examination report to recognize the prior art, the claimed technical advance and the exact statutory basis; and to make an objection other than that the application is evergreening.

Fifth, India should continue to have a public-health perspective in opposition/ post-grant review, provision of patent information and through careful analysis of claim scope. Research exemptions and other legal avenues for follow-on research should continue to be meaningful. Licensing models can be used to gain a balance between exclusivity and access when a claim is valid, appropriately limited and genuinely inventive. Refusal serves to preserve the integrity of the patent system and to ensure future competition if the claimed contribution is speculative or speculative in a manner not anticipated by section 3(d).

Conclusion

Although in-silico drug repurposing offers a gold mine of new therapeutic applications of existing drugs, the novelty of a drug is not synonymous with patentable invention. The protection against pharmaceutical

evergreening in India is a unique protection for new forms and derivatives of known drugs under section 3(d). Novartis is saying that only a genuine new indication that meets the statutory efficacy requirement can be claimed; it is not saying that all claimed new indications are unpatentable. In the U.S. method-of-treatment claims are considered patentable, subject to the general patentability requirements, while in China treatment claims are not patentable, but pharmaceutical-use claims are patentable subject to novelty, inventiveness and disclosure requirements.

The right way to do it is not to exclude AI-enabled repurposing from section 3(d) and not to treat it as 'bad'. Indian examination should focus on the specific claim category, evaluate the disclosure in terms of quality and extent, and utilize novelty and inventive step for the reasons for each. An evidence-sensitive, claim-specific, clear framework can prevent speculative monopolies from occurring while maintaining protection for substantial and valuable advances in therapeutics. This would allow patent law to evolve to respond to computational science, while retaining the public health values that are the heart of India's anti-evergreening policy.

REFERENCES:

1. Atlas Powder Co. V. IRECO Inc., 190 F.3d 1342 (Fed. Cir. 1999)
2. Ashburn, T.T. Thor, K.B., "Drug Repositioning: Identifying and Developing New Uses for Existing Drugs", Nature Reviews Drug Discovery, Vol. 3, 2004, pp. 673-683
3. Bhaven N., Sampat and Kenneth C. Shadlen, "Indian Pharmaceutical Patent Prosecution: The Changing role of Section 3(d)".
4. Bayer Corporation V. Union of India (2014) 60 PTC 277 (Del.)
5. China National Intellectual Property Administration, Patent Examination Guidelines, 2024
6. China, Patent Law of the People's Republic of China, 2020 (as amended)
7. Chong, C.R. & Sullivan, D.J., "New Uses for Old Drugs", Nature, Vol. 448, 2007, pp. 645-646
8. Cousions, H.C., Nayar, G. & Altman, R.B., "Computational Approaches to Drug Repurposing: Methods, Challenges and Opportunities, Annual Review of Biomedical Data Science, Vol. 7, 2024, pp. 15-29.
9. DiMasi, J.A., Grabowski, H.G. & Hansen, R.W., "Innovation in the Pharmaceutical Industry: New Estimates of R&D Costs", Journal of Health Economics, Vol. 47, 2016, pp. 20-33.
10. Ekins, S. & Williams, A.J., "Finding Promiscuous Old Drugs for New Users", Pharmaceutical Research, Vol. 28, 2011, pp. 1785-1791
11. Government of India, The Patents Act, 1970 (Act No. 39 of 1970), as amended
12. Government of India, Manual of Patent Office, Practice and Procedure, Office of the Controller General of Patents, Designs and Trademarks.
13. India, The Patents (Amendment) Act, 2005 (Act No. 15 of 2005).
14. Mullard A. "The Drug-Maker's Guide to the Galaxy", Nature, Vol. 549, 2017, pp. 445-447.
15. Nosengo N. "Can You Teach Old Drugs New Tricks ?", Nature, Vol. 534, 2016, pp. 314-316.
16. Novartis AG V. Union of India, (2013) 6 SCC 1.
17. Oprea T. et. al. "Unexpected Therapeutic Opportunities in the Human Genome", Nature Reviews Drug Discovery, Vol. 10, 2011.
18. Parvathaneni V. "Drug Repurposing: A Promising Tool to Accelerate the Drug Discovery Process", Drug Discovery Today, Vol. 24, No. 10, 2019, pp. 2076-2085.

19. Polamreddy P. & Gattu N. “The Drug Repurposing Landscape from 2012 to 2017: Evolution, Challenges and Possible Solutions” Drug Discovery Today, Vol. 24, No. 3, 2019, pp. 789-795.
20. Pushpakom S. et. al. “Drug Repurposing: Progress, Challenges and Recommendations”, Nature Reviews Drug Discovery, Vol. 18, 2019, pp. 41-58.
21. Roche V. Cipla, 2015 SCC OnLine Del 13619.
22. Shamnad Basheer and T. Prashant Reddy: “The Efficacy of Indian Patent Law: Ironing out the Creases in Section 3(d)”
23. Section 2(1)(j) of the Patent Act, 1970: “invention" means a new product or process involving an inventive step and capable of industrial application.
24. Section 2(1)(ja) of the Patent Act, 1970: "inventive step" means a feature of an invention that involves technical advance as compared to the existing knowledge or having economic significance or both and that makes the invention not obvious to a person skilled in the art.
25. Section 3(d) of the Patent Act, 1970: the mere discovery of a new form of a known substance which does not result in the enhancement of the known efficacy of that substance or the mere discovery of any new property or new use for a known substance or of the mere use of a known process, machine or apparatus unless such known process results in a new product or employs at least one new reactant.
26. Section 3(i) of the Patent Act, 1970: any process for the medicinal, surgical, curative, prophylactic diagnostic, therapeutic or other treatment of human beings or any process for a similar treatment of animals to render them free of disease or to increase their economic value or that of their products.
27. Tanoli Z. et. al. “Computational Drug Repurposing: Approaches, Evaluation of In Silico Resources and Case Studies”, Nature Reviews Drug Discovery, Vol. 24, 2025, pp. 521-542.
28. United States Congress, 35 United States Code, $$ 101, 102, 103 and 112.
29. United States Patent and Trademark Office, Manual of Patent Examining Procedure, $2106, “Patent Subject Matter Eligibility”
30. United States Patent and Trademark Office, Manual of Patent Examining Procedure, $2164, “The Enablement Requirement”.
31. World Intellectual Property Organization, Agreement on Trade-Related Aspects of Intellectual Property Rights (TRIPS), 1994.
32. World Intellectual Property Organization, “AI enabled Health Innovation and IP: From Idea to Impact”
33. Xue H. et. al. “Review of Drug Repositioning Approaches and Resources”, International Journal of Biological Sciences, Vol. 14, No. 10, 2018, pp. 1232-1244.