Patenting AI-driven drug compound screening inventions in China

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The integration of AI in drug discovery, particularly in the screening of drug compounds, ushers in seismic change to the pharmaceutical industry. AI technologies, especially machine learning and deep learning, have revolutionised how new drugs are identified and developed. The development of AI-driven algorithms fuels drug discovery from detecting and prioritising disease targets, identifying potential drug candidates within large chemical libraries, predicting molecular behaviour, to simulating clinical trial outcomes, which drastically shortens the process and brings down the costs.

For instance, a biopharmaceutical company, by leveraging AI platforms designed for drug discovery, managed to nominate ISM001-055, a drug candidate for idiopathic pulmonary fibrosis, with a budget of around $2.6 million within 18 months, in comparison with the usual tens of millions of expenditure incurred over several years.

A study in 2023 indicates that there are more than 70 AI-derived small molecules, antibodies, and vaccines currently in clinical trials. Although applications have been filed to patent these newly found drug compounds, patenting the algorithms associated with the finding of such compounds is not that straightforward. The rationale behind this is that the algorithms or programmes per se are prone to be deemed as “the rules and methods for mental activities” or “abstract ideas”, which is unpatentable subject matter in many jurisdictions, including China. On top of that, algorithms iterate at a fast pace, which could put the inventors in a quandary as to whether it is worthwhile to patent their algorithms at all.

Practice in China

The filing requirements for patent applications for AI-driven innovations in China remain the same:

- A claimed invention must be a statutory ‘invention’ in the sense that it is an eligible subject matter;
- The claimed subject matter must be novel and involve an inventive step (i.e., it is non-obvious); and
- The specification and claims must satisfy the following: enablement requirement/sufficient disclosure, and the claims

are supported by the specification.

As for AI-related methods, in general, a pure algorithm or piece of software per se is deemed to be unpatentable. However, if an algorithm or a piece of software is combined with a specific technical application, the combined technical solution may be deemed patentable. In the screening of drug compounds, if AI algorithms generate significant technical improvement or optimisation, such as increasing the accuracy and/or efficiency of screening, the technical solution may be patentable.

In prosecuting AI-driven inventions, inventors need to focus on whether the invention solves a specific technical problem and produces a technical effect. With regard to drug compound screening, it is pivotal to demonstrate how the existing drug discovery process is improved by the application of AI.

The 2023 version of the CNIPA's Guidelines for Patent Examination and the 2023 Comparative Study on AI-Related Inventions jointly conducted by the CNIPA and the JPO offer guidance on how to approach AI-related inventions by providing examples and explanations to help applicants to better understand how to construct their applications to meet filing requirements.

The extensive and in-depth application of AI across various fields and the new interdisciplinary techniques pose substantial challenges to the CNIPA. For instance, in the examination of an AI-driven drug discovery invention, the examiners will need expertise in both computer science and biology/pharmacy to understand how the two disciplines work in tandem to achieve the desired technical effect. This could markedly slow down the examination process.

For instance, Wanhuida's search of the CNIPA's official database indicates that a Chinese biopharmaceutical company that filed a dozen patent applications between 2019 and 2022 for AI-related pharmaceutical methods has so far received a first office action for only one application, with the rest still awaiting examination.

Over the past few years, though the CNIPA has granted a number of patents covering the use of AI in drug discovery (e.g., patents related to using AI to optimise the structure of a drug candidate molecule or to predict the effect of a molecule's interaction with a particular biological target), the number of patents granted for AI-related methods is far lower than the number of patents granted for screened compounds and the uses thereof.

Examples of CNIPA examination practice

The following examples offer a glimpse into the CNIPA's examination practice.

Patent CN114432311B relates to a drug compound for treating idiopathic pulmonary fibrosis and a computer method for predicting and screening the same. In this invention, 20 candidate compounds were selected for Collagen 1A2?A549 cellular validation testing after the first round of virtual screening and machine learning model prediction. The experimental data from these 20 candidate compounds was then fed back into the machine learning model. Combined with the results of the virtual computation, this process yielded nine candidate compounds in the second round. Following cell and animal experimental validation, two compounds with pharmaceutical activity were identified. Initially, the applicant sought to patent two compounds,

formulas I and II, and the computer method for predicting and screening. In responding to the CNIPA's office action, which stated that there was no unity among the three subject matters, the applicant opted to claim the compound of Formula II and abandoned the method.

Patent CN114839369B relates to microbial markers for acute high-altitude response and the applications thereof. In the patent, seven microbial species have been screened to be effective against acute high-altitude response using the XGBoost (eXtreme Gradient Boosting) machine learning method. The granted claims of the patent only include the above microbial markers and their applications, and do not cover the related machine learning methods.

Patent CN110352459B refers to a method for excavating a new drug candidate targeting nonstructure-structure transition site and apparatus for excavating a new drug candidate. Machine learning methods such as neural networks are used in the step of identifying a disorder-to-order transition region and other steps. All four granted claims involve the excavating method, and each step of the method is implemented by a computer device.

Patent CN113039559A proposes a training model that is a variational autoencoder with a learnable prior that is parametrised with a tensor train (VAE-TTLP). The model may be used to generate chemical structures that have desired properties. The VAE-TTLP model can also be used in combination with a reinforcement learning framework to expand the structure of the latent manifold (e.g., the latent space) towards novel chemical structures, such as novel inhibitors of protein or other biological activity. This patent application has not been allowed yet, but its chances are looking good, as the examiner acknowledged the novelty and inventive step of most dependent claims in the first office action.

Final thoughts

Due to the scarcity of case law and statistics, it would be too early to conduct any meaningful and systematic analysis of the CNIPA's examination practice concerning AI-driven drug compound screening. In principle, inventors are advised to focus on improving the transparency and predictability of AI systems to enhance their patentability.

As AI continues to evolve, intellectual property offices such as the CNIPA need to ramp up the recruiting and training efforts of interdisciplinary examiners and to further refine their guidelines to better address the challenges created by a talent shortage and technical hurdles.

It would also be advisable for stakeholders to keep abreast of the latest legislative and practical updates so as to navigate the constantly evolving landscape.