Artificial
Intelligence

Using AI for Drug Discovery – IP considerations

In this article, we take a closer look at patent protection in Europe for developments of AI in drug discovery. Many companies already use AI to aid the discovery of compounds that could potentially lead to new drugs, or to discover new uses for known drugs. AI has huge potential to disrupt this industry, where roughly 9 in 10 of every drug candidates fails to make it to market and where billions of dollars is invested for each drug that eventually comes to market. This article considers the different methods used and the IP considerations that users of AI should bear in mind.

How does it work?

There are many ways in which AI is used to aid drug development and discovery. The methods discussed below are merely a sample of the many ways of solving the problem of how to improve drug discovery.

BenevolentAI, a UK-based firm that recently announced a collaboration with AstraZeneca, aims to use AI at all stages of drug development, from discovery to late stage clinical development. This firm uses machine learning to mine and analyse biomedical information from clinical trials data and academic papers. The AI can then identify molecules that have failed clinical trials and predict whether those molecules would be more efficient in targeting other diseases. The predictive power of the AI can also be used to design new molecules. The collaboration with AstraZeneca is intended to discover new drugs for chronic kidney disease and idiopathic pulmonary fibrosis.

Atomwise is a company which approaches drug discovery from a very different perspective. It aims to find new molecules for diseases which have been hard to target, especially "undrugged" proteins, and has recently announced a partnership with Eli Lilly. Atomwise have applied methods for speech and image recognition to chemistry to predict the bioactivity of small molecules. Their technology is based on convolutional neural networks and extracts insights from millions of experimental affinity measurements and analysis of thousands of protein structures to predict the binding of small molecules to proteins.

Recursion Pharmaceuticals represents yet another radically different approach to drug development. They use high-throughput screening methods to generate hundreds of thousands of cellular images which their AI software analyses. The AI allows development of cellular models of diseases, which provide insights into toxicity, dose-response characteristics, and target discovery and prediction. Their entirely automated approach is more similar to traditional drug screening methods, but is scaled up to allow thousands of compounds to be screened against hundreds of diseases cheaply and quickly.

IP considerations – Patents

The compounds that are discovered are an obvious target for patent protection for any company using AI in drug discovery. In this respect, drugs are a good opportunity to get patent protection on products discovered via AI. BenevolentAI, for example, have several patent applications in their name which all appear to be directed solely towards the products of their AI (i.e., compounds and uses thereof).

Companies may also decide to use patents to protect their AI. Atomwise and Recursion Pharmaceuticals appear to have patent applications directed towards their AI, whereas BenevolentAI does not appear to have any pending applications which disclose their AI.

Patents, by their nature, require public disclosure of a company's methods or product. There is a possibility that by disclosing an AI for drug discovery would make any drugs resulting from that AI obvious, if for example it could be demonstrated that the AI would always arrive at the same result when given a problem and that a skilled person would inevitably arrive at that solution if he/she were given the problem and the AI. Anyone seeking to protect their AI should therefore take care that their disclosure of the AI does not render any drugs resulting from the AI obvious.

When considering patent protection, it is also important to remember that, in Europe, an invention must be directed towards a non-obvious technical solution of a technical problem. In this respect, all features which contribute to the technical character of the invention are taken into account. The EPO's guidance is that AI-related innovations should be described and claimed as being developed for a specific implementation. However, a pending Atomwise EP application has been deemed to relate to non-technical matter because the claim is "not sufficiently limited to ensure that [the] technical purpose is actually served by the distinguishing features over the whole claim scope". Applicants should therefore ensure the technical purpose is plausibly served across the whole scope of the claimed subject matter.

AI users may also consider using trade secrets to protect their AI. Trade secrets do not prevent third parties from independently arriving at the same solution, however, and anyone using trade secrets should also be aware of the dangers of third parties reverse-engineering their AI.

In summary, patent protection is available for AI technologies in the field of drug discovery and companies operating in this area should seek expert guidance at the earliest opportunity to discuss their options and any difficulties they may encounter.

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