Commentary

Can an artificial intelligence model be the inventor of a molecule designed by the model and how can patentability be assessed?

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1 Introduction

It appears not appropriate to refuse patentability of an invention on a new molecule designed by AI because the respective patent application does not have significant examples which were carried out in reality, but only generated by AI (usually a trained model/machine trained algorithm). However, to achieve patentability, certain requirements must be fulfilled, in particular relative to the estimation accuracy of the trained model and to successful repetition of the examples in view of known state of the art at the filing date.

It is more than questionable if an AI model can be the inventor of a molecule designed by the model, the first patent applications in this respect having been filed. Assessment of inventive step for new molecules generated by AI should remain subject of discussion. There are no clear positions by the patent offices for the time being.

It is a well-known fact that Artificial Intelligence (AI) has a vastly growing impact on our everyday life, for carrying out innovative and creative acts resulting in inventions, which could previously only be made by humans.

A rapid development in the use of computers in chemistry could be observed in the last 50 years. A further immense development, now in the design of new molecules, occurred when computers became powerful enough to process machine learning algorithms, discover patterns in data, and construct mathematical models using these discoveries. Algorithms can be provided with data to learn from (trained model). This is the principle of Artificial Intelligence. Patents can be issued on trained models themselves, or the trained model can be applied, e.g. in pattern or language recognition or the subject-matter of the present article – designing molecules (Chen et al., 2018; Engkvist et al., 2018; Sellwood et al, 2018).

Many questions relating to the protection of these inventions yet remain to be answered. The readers' attention is hereby drawn to the fact that the field "AI and patents" is still in a very early stage of development. Little is known. Only a limited number of publications related to this subject-matter exist, and it cannot be said that it is easy to get an overview on the actual state of art in the field. Some articles are very general, some treat the use of AI in drug discovery, some give general overviews of the various fields where AI can be applied, some disclose in which technical fields AI is used, and so forth.

The following publications are of considera-

ble interest in the present field:
"Artificial Intelligence and Drug Discovery" (Leanse, T., 2019)

"Artificial intelligence: the implications for patents" (Kuhnen, R. K., 2019)

"Artificial creativity—is the IP system ready for robot inventors?" (Inchley, T., 2019)

„Machine yearning: AI and patents" (various authors, 2019)

"Patenting Artificial Intelligence: Issues of Obviousness, Inventorship and Patent Eligibility" (Tull, S. Y. and Miller, P. E., 2018),

"WIPO Technology Trends 2019 Artificial Intelligence" (WIPO, 2019).

A frequently encountered question concerns not the patentability of an AI method as such, but of molecules, materials, compositions and the like, designed (conceived) thereby. In these cases, the human (i.e. the „classical" inventor) plays a lesser and lesser role. It is expected that this will have an impact on the assessment if results (examples) conceived by AI meet the requirements for sufficiency of disclosure.

It is assumed that AI is used frequently in chemical and pharmaceutical industry to design new molecules or related compositions of matter. However, it is not clear to which extent AI is used since industry is rather silent in this respect. Furthermore, the number of filed patent applications cannot be taken as an indicator. Due to uncertainty if protection of a molecule designed by AI (and not in the lab) is available at all, industry has not filed patent applications in this field. In surplus, the questions who is the inventor of the molecule and how the inventive step (i.e. if the new molecule is sufficiently distinct from the prior art) is assessed are not clear. As long as this is the case, patent applications will not be filed.

Hereinafter, it will be tried to give an answer to the question if it is or will be possible to patent molecules, materials, compositions and the like showing advantageous properties which are designed by AI and, in the affirmative, if the AI model is the inventor of the new compound. The author will furthermore address some crucial questions relating to the assessment of the inventive step.

2 Patentability of molecules designed by artificial intelligence

In the present context, molecules having pharmacological activity (interaction with targets, e.g. antigens, antibodies, enzymes) play a paramount role. However, the results provided below also apply for materials, compositions and the like not having a physiological, but other activity.

In the context of the present article, the term "molecule" refers not only to molecules, but also to materials, compositions and the like including DNA, enzymes, antibodies, (liquid) crystals, just to name a few.

The interaction of molecules with certain targets can be calculated very accurately today using AI. Even though this is nothing else, in principle, than well-known „*in silico chemistry*", calculations supported by AI ("trained model") now have a more accurate scientific basis, generating in many cases precise results in shorter time.

In consequence, an actual question in this respect is whether „AI-generated" ("trained model generated") molecules having certain (alleged) properties can be patented as such, even though they were not synthesized and tested in vitro at the priority date.

To answer this question, the two decisive questions criteria should be:

1) Does a patent application on a molecule generated by AI provide ample disclosure in the description and the (not real) examples for the person skilled in the art to enable

synthesis of the respective molecule in vitro?

2) Does the skilled person, at the priority date, assess the examples (and the respective parts of the description) as credible, because they do not contradict common teachings and/or the estimation accuracy of the trained AI model is sufficiently high?

It is held that application of the above two criteria could serve to avoid that the examples in the respective patent application are just an (uneducated) guess not having a sound scientific basis (meaning that even if the examples of the application could be successfully reproduced, this was purely accidental).

The above approach is supported, on the one hand side, by the **Japanese Patent Office JPO**, in "Examination Guidelines for Patent and Utility Model" (JPO, 2019a), „Case examples pertinent to AI-related technology" (JPO, 2019b) and „Newly Added Case Examples for AI-Related Technologies" (JPO, 2019c) (Presentation Material).

Example 51 in "Case examples pertinent to AI-related technology" and „Newly added case examples for AI-related technologies" is a fictive example for a patent application not providing enabling disclosure. The application is on a curable adhesive invented by a trained AI model. The adhesive has a certain composition to cure faster than state of the art adhesives. No real examples are found in the description, only an example created by the trained model. The estimation accuracy of the trained model has not been verified.

The facts that a) it was common technical knowledge at the priority date that it is difficult to control the curing reaction the way described in the patent application; and b) the example is a "trained model example" created without a verified estimation accuracy, are reasons that the application is assessed as not providing enabling disclosure (written support) in the description. This cannot be remedied by later filing data showing that the trained model result was correct, as the skilled person would not have believed that the claimed invention can be carried out at the priority date, for being a) contrary to common knowledge and b) based on speculation. However, this conversely should mean that the invention would have been patentable if the two above criteria had been met.

The actual „Guidelines for Examination" of the **European Patent Office EPO** answer almost exclusively questions related to assessment of inventive step and technicity of AI methods (Guidelines for Examination in the European Patent Office, November 2019, Section G-II, 3.3.1, Section G-II, 3.6, G-VII, 5.4) (EPO, 2019). Unfortunately, support for the correctness of the above assessment is not found there.

Such support, however, appears to exist in case law of the Boards of Appeal of the EPO. It is pointed to case law on so-called „prophetic examples", which are established as proof to show that an invention can be carried out at the priority date. Definite proof can then be filed at later points in time by "real" examples. However, in general such proof is only accepted if the teachings of the claims and the description is not contrary to the general teachings in the particular field at the priority date. Decisions have to be taken on a case-by-case basis.

In the present context, the decision T2220/14 (EPO Boards of Appeal, 2015) backed up by T1496/08 (EPO Boards of Appeal, 2012), is worthwhile mentioning.

T1496/08 states the following (p. 20, 1st paragraph): "*Post-published evidence may be taken into account,* ***but only to back-up the findings in the patent application*** *in relation to the use of the ingredient as a pharmaceutical, and not to establish sufficiency of disclosure on its own."* T2220/14 states the following in Point 63. of *"The Reasons for the Decision": The respondents have not presented convincing evidence that this would be the case, their main argument being that Example 3 is a "prophetic" example. However,* ***there is no requirement in the EPC that, either at the priority or filing date, the applicant must have carried out the*** claimed

invention. *The requirement of Article 83 EPC is that a person skilled in the art, following the* ***teachings in the application*** *as filed supplemented with his/her* ***common general knowledge*** *and with a reasonable amount of experimentation, including* ***some trial and error,*** *would be able to carry out the invention as claimed at the relevant date.* (emphasis added).

In summary, it appears not appropriate to refuse patentability of an invention on a new molecule because the respective patent application only has AI (trained model) generated examples. This would be the same as refusing an invention on a new molecule because all examples are prophetic. As shown by the Guidelines for Examination of the JPO and the above EPO case law, this is not appropriate – it has to be checked if the examples can be successfully carried out and – in the affirmative - if the success was not accidental. To this end, it has to be verified if the examples are not in line with common knowledge at the priority date and if the estimation accuracy of the trained model is sufficiently high.

3 Inventor questions

Another crucial question is: who is the inventor of molecules designed by AI? The person who has created the trained model and/or who has applied the trained model to find the new compounds? According to generally applied principles, an inventor must be a natural person (it should be noted, however, that this is not explicitly required by the European Patent Convention). However - what to do when an invention has been clearly made by a machine trained algorithm? Until now, for "serious" inventions having a potential commercial value, no one will name the trained model as an inventor, because it seems clear that the application will be rejected for not complying with inventor requirements.

However, recently two patent applications were filed in various countries by the same applicant (Dr. Stefan Thaler) which have in the meantime been published under the numbers EP 3 564 144 und EP 3 563 896 by the EPO . A machine trained algorithm was named as the inventor. The algorithm as such appears to be protected by a patent application (US 2015/0379394), naming Dr. Stephan Thaler as an inventor. The subject-matter of the patent applications are a food container and an electronic device.

More information is available on the website of the EPO (EPO, 2019), the magazines "The IPKat" (Hughes, 2019a, 2019b; Papadopoulou, 2019) and "iam" (Wild, 2019). This case should be a "trial balloon" challenging the Patent Offices to give an answer to the crucial question if a trained model can qualify as an inventor.

4 Inventive Step

A further, important topic, frequently also encountered when molecules are designed by AI is the inventive step. "Inventive Step" or also "Obviousness" refers to the patentability criterion if the new invention is sufficiently remote and different from what is known in the art (the pool of publications in the same field) is not considered "trivial".

Let's take the case that an individual helps to create a trained AI model/machine trained algorithm. The model reveals to give excellent results in designing molecules having certain desired properties, e.g. binding to certain targets (e.g. enzymes, receptors in the medical field) or lending themselves as perfuming ingredients, colorants or sweeteners, just to name a few. The person having conceived the trained model is the inventor, in the classical sense, of the model; but also (very probably, see below) of the new molecule. Until here, the story is still easy. But how about the assessment of the inventive step if the same model is used again to design further molecules? It appears that the threshold for patentability relative to inventive step becomes higher, or that the in-

ventive step will be even denied. The design of a new molecule using the same model which has been already successfully applied in the design of the first molecule could be regarded as a simple routine act, even though the specific molecule provides advantageous properties and would be regarded as inventive under "classical" criteria.

It is not clear if one day the respective Patent Offices will take the above approach. In any case, applicants wishing to patent new molecules designed by AI may prefer not to disclose that the "method behind" the creation of the new compounds is a machine trained algorithm, in order not to "raise the bar" for the inventive step or, rather, to have the examiner apply the "classical" criteria. Applicants may even think of not disclosing the model in the first application (in which the trained model was used for the first time), i.e. not to mention the model. In this respect, however, the question arises if it does not become evident that the new molecules were the result of a trained model and the application gets rejected for lack of disclosure. The AI used to design new molecules should in principle be open to protection by patents. Such exclusivity for the best AI would clearly provide the company, often a drug company, with a competitive advantage. However, the protection for molecules, and in particular the important "crown jewels", might get lost, in a worst-case scenario.

5 Discussion

As more and more new molecules are designed by AI, without any examples having been carried out in vitro, the question arises if the design of the particular molecule results in a patentable invention. To answer this question, it appears appropriate to use argumentation based on patents having prophetical examples (the other type of examples which have not been carried out when the patent application was filed). Since patents having prophetical examples can be granted under certain conditions, this should also apply for patents having only examples for AI-designed molecules. A careful analysis of the Guidelines for Examination of the JPO and the above-cited EPO case law (EPO, Guidelines for Examiniation) reveals which criteria for patentability should be checked if the examples can be successfully carried out. It should be verified if the examples are in line with common knowledge at the priority date and if the estimation accuracy of the trained model is sufficiently high. Then the success was not accidental.

It seems that the bar for patentability of compounds designed by AI will inevitably be raised. Many questions cannot be answered for the time being, one of them being if AI programs can be inventors. Two cases are known to date in which patent applications naming an AI inventor have been rejected by the European Patent Office (decision can be appealed). As the reasoning for the decisions is not available yet, it is not clear what is behind the decision, but it is assumed that the EPO will base it on the reason that the inventor is not a human being.

It is not clear how the inventive step will be assessed in case an AI-designed compound was found patentable and the same trained model shall be used again to design a (further) compound. In such a case, the examiner may argue it was known that the trained model is capable of successfully designing new molecules with some desired properties. The design of another molecule will then just be the result of a routine act, namely providing the relevant data to the model. At present it is not clear how such an objection can be avoided or overcome. One solution might be not to disclose that the molecule was designed by a machine trained algorithm. This should avoid the objection that the new molecule was created in a routine act. However, shouldn't it immediately become obvious that the examples are only based on AI? Maybe this does not even trigger negative consequences as after all the situation appears very similar to a "classical" pharmaceutical patent application with prophetic examples

(which would correspond to the AI-generated examples). Yet this would mean that the subject-matter of the application is patentable!

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