

AI in Chemistry and Patent Law: Current and Future Issues



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Topics

- What is AI?
- Applications of AI in chemistry
- AI-generated prior art
- AI and inventorship

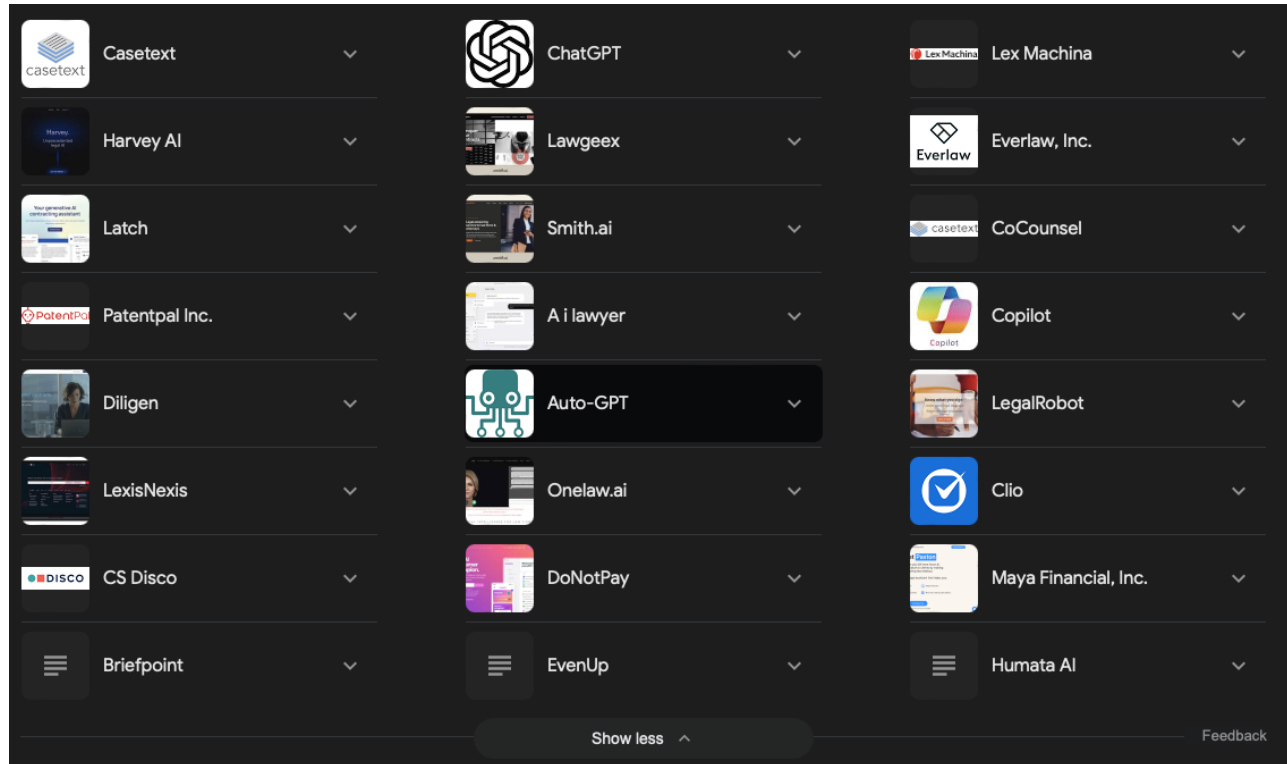
What Is AI?

- Technology that enables computers to simulate human intelligence and problem-solving capabilities.
- A large language model (LLM) enables computers to achieve language generation and other natural language processing tasks such as classification.
- Can be “multimodal”
 - Input/Output do not have to be language
 - Video, image, audio, text, chemical structures, 3D movement
- Future: Artificial general intelligence (AGI) is a type of AI that matches or surpasses human abilities across a wide range of cognitive tasks.
- Future: Artificial superintelligence (ASI) is a type of AI with intellect far beyond human intelligence.

How Can AIs Be Useful Today?

- LLM AIs predict what a person would do, based on the materials used to train it.
- Although some current AIs approach the abilities of an average human being in specific areas, the current sentiment is that we have not yet accomplished artificial general intelligence (AGI) which would require human-like performance in all areas.
- Even with these limitations, current AI can be a powerful tool, as it can do the work of many average-skill human beings in a short time with essentially no human labor required.
- Scientific research and discovery is ultimately composed of many simple tasks that can each require an enormous amount of human labor and time, but that do not necessarily require super-intelligence or even a high degree of training to carry out.
- AIs are poised to make scientific research and discovery much more efficient. AIs can rapidly perform simple tasks that would take a significant time for 1, 10s, 100s, or even 1000s of people to perform.
- AI development is rapidly evolving and generating an enormous amount of commercial interest.

AI Tools for Lawyers



Special Considerations for AI Tools for Lawyers

- Must keep confidential information private and secure!
 - Note that many general AI tools do not do this!
- AI should be trained in the specific legal area where used.
- Answer quality must be high, with minimal or no errors or hallucinations.
 - Should include references to source documents whenever possible.
- Needs to be user-friendly.

AI Tools for Patent Examiners

- Announced 2/1/2022: “More like this” feature in Patents End-to-End (PE2E) Search tool.
 - Uses AI algorithms to generate a list of domestic or foreign patent documents that are similar to a specific patent document.
- Also part of 2/1/2022 announcement: In addition, the USPTO is in the process of developing and testing other AI search capabilities for future integration with PE2E search, such as AI features that:
 - Generate suggestions for prior art references
 - Refine document sorting
 - Add insight into AI reasoning
 - Provide additional Cooperative Patent Classification suggestions

AI in Chemistry

An abstract graphic in the background consisting of a network of glowing blue and green lines connecting various points, resembling a molecular structure or a data network. The lines are thin and the points are small dots, creating a complex, interconnected web.

AI Tools for Organic Synthetic Chemists

- Spaya from Iktos
- IBM Rxn
- AIzynthFinder (open-source)
- Synthia (was Chematica) from MilliporeSigma/Merck
- SynAsk
- ChemCrow from IN SILICO CHEMISTRY
- Molecule.one
- Pending.ai
- ChemAIRS from Chemical.AI
- Reaxys from Elsevier
- SciFinderⁿ from CAS

Journals About AI in Chemistry



- Example article: Rizvi Syed Aal E Ali, Jiaolong Meng, Muhammad Ehtisham Ibraheem Khan, Xuefeng Jiang, “Machine learning advancements in organic synthesis: A focused exploration of artificial intelligence applications in chemistry”, Artificial Intelligence Chemistry, Volume 2, Issue 1, 2024, 100049, ISSN 2949-7477.

Current Applications of AI in Chemistry

- What can AI do in chemistry?
 - Literature review
 - Proposing synthetic routes to target compounds
 - Laboratory synthesis of target compounds (e.g., with use of robotic laboratories)
 - Screening of target compounds (e.g., early-stage identification of promising candidate compounds based on ease of synthesis, potential activity against a target, and/or actual activity against a target)
 - Characterization/analytical chemistry (e.g., interpretation of spectra, proposing analytical methods for complete characterization of compounds)
 - Data analysis
 - Writing up results

AI in Drug Discovery: Drug Design

- Identifying biological pathways implicated in specific diseases
- Identifying potential biological targets for disease treatment
- Prediction of new bioactive compounds or new uses for known compounds
- Predicting efficient synthetic routes toward a target compound, and/or selection of candidate compounds that can be efficiently synthesized (e.g., low cost, scalability, green synthesis, or other efficiency considerations)

AI in Drug Discovery: Pharmacological Screening and Clinical Trials

- Screening
 - Automated high throughput screening against a target
 - Identification and optimization of lead compounds
- Predicting drug properties (e.g., based on literature review, computational chemistry, or comparison to known compounds)
 - Solubility
 - Bioavailability
 - Toxicity
 - Prediction of drug-drug interactions
- Analyze clinical trial data (e.g., finding and characterizing patterns in data)

AI in Drug Discovery: Companies Specializing in AI Drug Discovery

- Exscientia
- Standigm
- Genesis Therapeutics
- Data2Discovery
- Unlearn.AI
- Recursion
- BenevolentAI
- Xbiome
- Insilico Medicine
- Xilis

AI in Drug Discovery: Recent Examples

- Insilico Medicine: Developed 18 preclinical candidates since 2021 (in under 3 years).
- 5/25/2023: Insilico Medicine announced FDA investigational new drug (IND) approval for AI-designed ISM3091, a small molecule inhibitor of USP1 for potential treatment of solid tumors.
- 4/24/2024: Insilico Medicine announced FDA investigational new drug (IND) approval for AI-designed ISM3412, a small molecule inhibitor of MAT2A for the potential treatment of MTAP deleted cancers.
 - Insilico launching Phase I study in human subjects with advanced and metastatic solid tumors.

Scientific Goals Falling Within Chemical Arts

- Drug discovery
- Materials/compounds/polymers having specific desired properties.
- “Ultimate” scientific goals
 - Cold fusion
 - Curing cancer/disease
 - Preventing/slowing aging
- Hypothesis: Current or future AIs (e.g., AGIs, ASIs) could contribute to or do the brunt of the work in important future discoveries within the chemical arts.

AI-Generated Prior Art



AI-Generated Prior Art

- AI-generated prior art
 - AIs can generate documents that can be published, such as papers, patent applications, or searchable internet publications
 - AIs can generate false or “hallucinated” information
 - AIs can generate lots of information with little human labor
- AI-generated chemical prior art
 - Chemical structures and properties
 - Synthetic methods
- New AI developments
 - AI integrated into OS
 - Windows “Co-Pilot”. Apple “Siri”.
 - AI integrated into word processing software
 - Hypothesis: Some degree of AI-assistance is or will be a component of everything that humans publish.
 - Future?: AIs will help with or do a great deal of the work in scientific discovery?

USPTO and AI-Generated Prior Art

- 4/30/2024: Request for Comments Regarding the Impact of the Proliferation of Artificial Intelligence on Prior Art, the Knowledge of a Person Having Ordinary Skill in the Art, and Determinations of Patentability Made in View of the Foregoing.
 - Comments due 7/29/2024 (Submissions appear to be private)
 - "Listening session" held 7/25/2024 (Can view/listen to this now)
 - Prior art is presumed to enable the public to make and use the disclosure. Should AI-generated prior art be afforded such a presumption, or should it be treated differently?
 - Person having ordinary skill in the art ("PHOSITA")
 - Does PHOSITA need to be a natural person?
 - Should skill level of PHOSITA be moderated in view of the availability of AI systems?

USPTO Request for Comments on AI-Generated Prior Art: Enablement

- Prior art is presumed to enable the public to make and use the disclosure.
- The USPTO's Request seems to restrict the inquiry to "AI-generated disclosures (that have not been prepared and reviewed by a human)."
- Does this implicitly acknowledge that AI-assisted (human + AI) publications should be subject to normal prior art rules?

It Could Be Problematic to Treat AI-Generated Prior Art Differently than Other Types of Prior Art

- Hypothesis: AI will likely soon be a component of everything published.
- It is or may become difficult to quantify the degree of AI-assistance. It could be difficult to determine whether a human participated at all, or to what extent a human participated, in the preparation and review of a document.
- Is simple human review of a document with little or no changes sufficient to make the document not “AI-generated prior art”?
- If dramatically different treatment occurs for AI-generated prior art, lots of time/energy may get spent on the determination of whether a reference is AI-generated.

AI-Generated Prior Art: Enablement?

- Enablement/operability = Can a person having ordinary skill in the art make and use what is disclosed?
- The effect of the prior art on someone reading it seems like it should be more important than how the document was generated.
- Rebutting: If there is no enablement of a cited reference, the presumption of enablement of of the reference can be rebutted.
- If an AI can generate an enabling document, then there is no reason that this document should be treated differently than a human-generated document.

AI-Generated Prior Art: Enablement?

- MPEP 2121.02 Compounds and Compositions
 - One of ordinary skill in the art must be able to make or synthesize
 - To rebut presumption, Applicant can supply facts showing that a process for making was not known.
 - A reference does not contain an “enabling disclosure” if attempts at making the compound or composition were previously unsuccessful.
- MPEP 2121.03 Plant Genetics
 - Those of ordinary skill must be able to grow and cultivate the plant
- Properties of compounds/compositions
 - Inherency: Is the compound/composition enabled? If not, properties cannot be inherent from the reference.
 - For properties listed for non-enabled compounds/compositions, can argue the properties are not enabled either. This may be rebuttable if computational or other reasoning is given for the properties.

AI Impact on Skill Level of PHOSITA?

- If AI tools are customary for a PHOSITA, then does it make sense to adjust the skill level of PHOSITA upward to reflect this?
 - Adjusting skill level of PHOSITA in a technical area upwards may increase the difficulty of obtaining patents in that technical area.
- However, current AIs at best only duplicate/predict what a human would do. Only access to AIs with super-human intelligence, which do not yet exist, would meaningfully change the skill level of a PHOSITA.
- Therefore, current AIs should not change skill level of PHOSITA.
- Even the development of AGIs should not change this logic.
- However, in the future, as AIs get “smarter” (e.g., ASIs), this issue may need to be reevaluated.

AI and Inventorship



AI Cannot Be an Inventor on a US Patent

- On appeal, the Federal Circuit affirmed in *Thaler v. Vidal*, 43 F.4th 1207 (Fed. Cir. 2022) the holding “that only a natural person can be an inventor, so AI cannot be.”
 - The court stated that 35 U.S.C. 100(f) defines an inventor as “the *individual* or, if a joint invention, the *individuals* collectively who invented or discovered the subject matter of the invention.” (emphasis in original)
 - Based on Supreme Court precedent, the word “individual” when used in statutes ordinarily means a human being unless Congress provided some indication that a different meaning was intended.” Therefore, an inventor must be a natural person.
- Note that the court was not confronted with “the question of whether inventions made by human beings with the *assistance* of AI are eligible for patent protection.” (emphasis in original)

USPTO Guidelines on AI-Assisted Inventions

- Published 2/12/2024
- Inventors must be natural persons, even when AI has been “instrumental in the creation of the claimed invention.”
- AI-assisted inventions are not “categorically unpatentable for improper inventorship.”
- Although an AI system cannot be named as an inventor, “an AI system—like other tools—may perform acts that, if performed by a human, could constitute inventorship.”
- Patent protection may only be sought for inventions “for which a natural person provided a significant contribution” (emphasis added). A natural person must provide a “significant contribution” to each claim.

AI and Creation of Inventions: Future?

- As AIs become more capable (e.g., AGI, ASI), less human assistance will be needed to produce a patentable invention.
- AIs do/will have the ability to review portions of (or all of?) the literature, run experiments in robotic chemistry laboratories, and generate data.
- AI assistance will become the norm
 - With writing
 - With data analysis
 - With literature review
 - With experimentation?
- At some point, AIs may originate inventions from simple non-inventive prompts!

Future: Could the USPTO's Significant Human Contribution Standard Put AI-Assisted Inventions at a Disadvantage?

- Consider a scenario in which an AI-assisted invention could be patentable other than lack of a human inventor, while if a human discovers the same invention it is patentable.
 - Even if what the AI has done would be enough for patentability if a human had done the same thing, more human involvement could be required to satisfy human inventorship standard.
- For an entity seeking patent protection of their AI-assisted discoveries, could the USPTO's significant human contribution be characterized as anti-AI and as disincentivizing or punishing "heavy" use of AI in scientific research?

Could We Lower The Significant Human Contribution Standard?

- Allowing humans who contributed little to be inventors.
- May have adverse effects?
 - Could degrade the normal standard of inventorship.
 - If the determination of who is an inventor of a patent becomes less definite, this could severely impact the potential value of patents.

USPTO Guidelines on AI-Assisted Inventions: Prompt-Drafters and AI-Makers/-Trainers as Inventors?

- Prompt-drafter can be an inventor, in certain cases:
 - A natural person “who only presents a problem to an AI system may not be a proper inventor or joint inventor of an invention identified from the output of the AI system” (emphasis added)
 - “However, a *significant contribution* could be shown by the way the person constructs the prompt in view of a specific problem to elicit a particular solution from the AI system.” (emphasis added)
- AI-maker/-trainer can be an inventor, in certain cases: “The natural person(s) who designs, builds, or trains an AI system in view of a specific problem to elicit a particular solution could be an inventor, where the designing, building, or training of the AI system is a *significant contribution* to the invention created with the AI system.” (emphasis added)

Prompt-Drafters and AI-Makers/-Trainers as Inventors?

- The prospect of the AI-maker/-trainer as inventor may incentivize entities to make the investments needed for development of specialized AGIs or ASIs that can assist with or even originate discovery needed for significant scientific advances.
- AI system designers vs. AI system users: future contracts issues?
 - AI system designers may demand from users of AI systems partial ownership of inventions created by the AI system.
 - AI system users may demand from AI system designers that any patent ownership of inventions created by the AI system be assigned to the user.
 - For extremely powerful AI systems, this negotiation could become quite important.

With Better AIs, Will There Be Pressure to Make the Prompt Sufficient For Inventorship?

- Prompt-drafter can be an inventor, in certain cases:
 - A natural person “who only presents a problem to an AI system may not be a proper inventor or joint inventor of an invention identified from the output of the AI system” (emphasis added)
 - “However, a significant contribution could be shown by the way the person constructs the prompt in view of a specific problem to elicit a particular solution from the AI system.”
- What if future AIs become so “smart” that simple non-inventive presentation of a problem to an AI is enough to cause the AI to generate an invention?
 - If using an AI creates no inventorship in the user, this might disincentivize the use of AI-assistance in scientific discovery by entities that are not AI-makers/-trainers.
- Could more complex prompts than needed be intentionally used to ensure a significant contribution is made in the prompt?
- Could prompt-drafters intentionally design prompts to cause the AI to leave something out for a human inventor to later fill in?

Future: What Happens to Inventorship If/When ASIs are Created?

- If ASIs are created such that simple presentation of a problem to an AI is enough to cause the AI to generate an invention, a traditional user/purchaser of the software may not be needed for the ASI to create valuable inventions.
- Despite the possibly bizarre effects on inventorship, there are powerful arguments that the creation of ASIs should be incentivized for the betterment of humankind.
 - If humankind has the ability to advance itself into a new and better technological age, then they should do it.
 - e.g., achievement of cold fusion, cures for cancers/diseases, slowing aging, or achievement of other “ultimate” scientific goals could result in huge public benefits.
- In such a future, how can traditional commercial technology entities be incentivized to perform scientific research/discovery without the reward of a patent? Would all commercial technology entities become AI-makers/-trainers? Would all research/development be predominantly performed by ASIs?

Closing Statements

- Current AI has not achieved AGI or ASI.
 - Current AI cannot exceed what one or more average human beings could do, given enough time.
 - Therefore, the current legal framework which is designed to function with human-generated prior art and human inventors is likely sufficient to deal with current AIs.
 - The achievement of ASI may be a long ways away, but this is not certain.
- However, if/when AGI or ASI becomes widely available, skill level of PHOSITA may need to be raised to reflect this.
- To encourage the use of AI in scientific research, the USPTO could offer more clarity on what is required for prompt-drafters and AI-makers/-trainers to make a significant contribution.
- As AIs become more capable, we are likely to see creative prompt-making techniques, as well as increasing attention on contracts between AI-makers/trainers and AI system users regarding ownership of patents toward AI-assisted inventions.
- If ASIs are created, this could radically change the inventorship landscape such that AI-makers/-trainers are the predominant inventors of patents.

Thank you for your interest.

Questions?

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