Using Patents to Assess the Novelty of AI-Generated Drugs

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Artificial intelligence (AI) has created new opportunities for drug developers. In fact, drug developers claim that AI allows them to discover drug candidates that are particularly novel scientifically, with the potential for therapies that work differently than existing drugs. The question of whether AI-generated drugs are more novel than their traditionally-developed counterparts is important not only for industry and for patients but also for assessing legal questions involved in patenting and regulatory oversight of these drugs.

In this paper, we develop data analytic techniques to identify relevant molecular structures in patents, extract them, and determine novelty. Our preliminary results show that the average AI-generated drug is *not* more novel than controls. After completing our analysis of novelty, we next plan to use our dataset to answer questions about how firms select drug candidates to move from the lab to clinical trials and how patent examiners review patents with these structures.

Analysis of molecular structures in patents is widely used in the natural sciences; indeed, patents are one of the largest and most important inputs for chemical and biological databases. But molecular structures in patents have, to our knowledge, not been analyzed empirically at scale by legal scholars and are rarely used by economists. Our data science approach may therefore spark additional interest and future work in this area.

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