WILL ARTIFICIAL INTELLIGENCE (AI) REPLACE CHEMISTS?

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ABSTRACT

The current discussion surrounding the role of artificial intelligence (AI) in chemistry often centers on the provocative question of whether AI will supplant chemists in the laboratory. Such debates, while stimulating, tend to overshadow a more pressing and realistic consideration. At present, there is little evidence to suggest that AI will replace experimental chemists in research laboratories in the foreseeable future. However, a critical aspect frequently overlooked in these discussions is the competitive advantage that AI confers. Chemists who adeptly integrate AI into their research methodologies are likely to surpass their peers who do not adopt these advanced tools. This shift in research dynamics underscores the importance of embracing AI not as a replacement but as a powerful ally in the evolving landscape of chemical research. This article was written to demystify the capabilities and limitations of AI in modern chemical research, and to provide a balanced perspective on how AI tools can be effectively integrated without wasting the essential human element in scientific discovery.

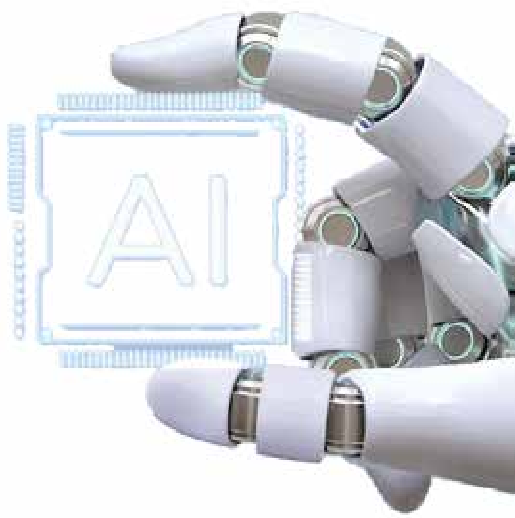
KEYWORDS:
- Artificial intelligence
- Chemical science
- Machine learning
- Chemical industry
- Chemical research

AI is one of the most rapidly developing technologies invented by humans, with a significant impact on science and technology. Chemical science has also been strongly influenced, witnessing unprecedented acceleration in various research fields (1, 2, 3, 4). The connection with robotics and automation is considered a prelude to an artificial intelligence laboratory and the autonomous synthesis of organic molecules (5, 6, 7). Structure elucidation is a long-term goal (8), where important steps, for example, include analyzing and interpreting microscopy (9) and spectroscopy data (10) with machine learning in real-time experimentation and proceeding to a 4D description of chemical phenomena (11).

However, it should be noted that AI is still far from being able to replace humans in laboratories. Synthetic chemists undergo extensive education and training to become "all in one" professionals. This training covers designing experiments, running optimizations, synthesis and separations, spectroscopy and analysis, purification and the effects of trace impurities, batch-to-batch variations of chemicals, and serendipity discovery, among many other areas. Most importantly, they are trained to find solutions when known knowledge and hints do not work. In many of these stages, AI has already become a valuable assistive technology. However, it is too early to expect a standalone AI, without human supervision, to synthesize a wide range of organic molecules with ease of use and acceptable running costs (12). Despite impressive progress, it is premature to think that computer-aided synthesis has solved all challenges (2).

It is extremely important that experimental chemists, over years of trial-and-error, gain knowledge about what does not work. This experience is often intuitive and is not easily shared. Indeed, the absence of negative experiments as training data is one of the key limitations for the development of AI models in chemistry (13).

Advanced AI-Chemist models still operate based on information available in existing knowledge domain and design/perform experiments using known techniques. Progress in the future significantly depends on human scientists (5). Several important areas of application for AI-driven technologies are explored in chemical engineering (14) and sustainability (15). While the advantages of AI in improving process development and reducing costs are unquestionable, on-site implementation requires an additional cognitive layer in the context of practical chemical production (16).



Progress may be reached in the distant future, but expecting AI to replace humans in research laboratories is currently too early. Yet, many outstanding AI tools already exist for chemical research, and these deserve closer examination.

From my personal experience, I first entered a research lab in the 1988-90s as a training pupil for chemistry Olympiad. At that time, computers had just entered regular chemistry laboratories. Difficult to believe, but many professional chemists considered learning computers a waste of time, preferring the "classical" style of the former period (articles were written on typewriters, and formulas were drawn by hand). Futuristic-minded researchers discussed that computers would soon replace chemists in labs, which eventually did not happen, as we clearly see now. However, those chemists who adapted to the computer era by upskilling to new tools quickly outperformed their slower colleagues in terms of productivity and efficiency. Even within a short period, the difference between those who immediately used computers and those who did not, became dramatically large. Currently, computers are a prerequisite in all laboratories.

The AI revolution in chemistry is already occurring and will significantly change research practices. Nevertheless, with all the optimism, the nearest goal is not to replace the experimental chemist in the laboratory, a task unlikely to be achieved soon. In contrast, as a point often missed in many overheated discussions, the nearest goal is the proper integration of AI-driven tools and solutions into synthetic practice. Following the example with computers, AI will not replace chemists, but those chemists who quickly adopt novel AI opportunities will inevitably replace those who do not. The near future lies in suitable digital training (17), increasingly integrated machine intelligence, and the balanced and accurate use of AI in chemical laboratories. This includes addressing issues of data and code availability, reproducibility of AI models, ethical issues, and guidelines for the publication of AI research, to name a few. Helpful AI is welcomed in chemistry labs!

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