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Editorial: Harnessing the Power of Large Language Model-Based Chatbots for Scientific Discovery

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With its ability to comprehend vast amounts of information, process complex data, and generate insights that were previously difficult to attain, ChatGPT and various other Chatbots are anticipated to have great potential for revolutionizing scientific discovery. First, ChatGPT can streamline the scientific discovery process by quickly sifting through the vastness of the scientific literature and identifying key findings, which saves the time of researchers and allows them to focus on interpreting the result and formulating new hypotheses.[1] By seamlessly integrating with existing research tools and scientific databases, ChatGPT can serve as a powerful assistant, making scientific discovery more effective.[2]

Second, researchers can collaborate with ChatGPT to design effective therapeutics.[3] On the one hand, by inputting the detailed data for the disease/target, ChatGPT can generate compound structures that have a high likelihood of clinical success; on the other hand, ChatGPT can predict the interactions between these compounds and their targets, providing researchers with a deeper understanding of how they function.[3] Third, ChatGPT can also greatly facilitate the advance of material sciences (building structures, writing codes for material software tools, etc.)[4] and chemistry (predicting the outcomes of different chemical reactions, suggesting new molecules that can be synthesized together with the potential route of molecular synthesis, etc.).[5] However, we note the potential pitfalls associated with the use of Chatbots, such as possible security threats and issues with copyright, privacy, misuse, bias, transparency, and incorrect or wrong answers.

To foster further discussion on the appropriate applications of Chatbots to diverse topics in pharmaceutical sciences, material sciences, biological sciences, chemistry, *etc.* (including but not limited to the design of effective therapeutics, the construction of novel materials, the prediction of chemical reaction outcomes, the synthesis of chemicals, *etc.*), *Journal of Chemical Information and Modeling* (JCIM) is announcing the publication of a virtual special issue on the topic of **Harnessing the Power of Large Language Model-Based Chatbots for Scientific Discovery**.

We invite submissions from researchers and scientists worldwide to report on the applications of Chatbots for promoting scientific discovery. We welcome all types of manuscripts that fit the scope of JCIM, such as articles, perspectives, viewpoints, reviews, letters, and application notes. Please find more information on the manuscript type at JCIM's official site.

Please note that we are not inviting papers written by large language model-based chatbots but, rather, papers that used that technology in applications and/or their research workflow. To ensure editors, reviewers, and readers understand the potential impacts of AI-generated content, current ACS policies state that "The use of AI tools for text or image generation should be disclosed in the manuscript within the Acknowledgment section with a description of when and how the tools were used. For more substantial use cases or descriptions of AI tool use, authors should provide full details within the Methods or other appropriate sections of the manuscript". More information about ACS guidance for AI tool use in manuscript preparation can be found here: https://publish.acs.org/publish/authorship_guidance_policies.

We are requesting interested authors to submit their manuscripts by August first, 2024. Submissions will be peer-reviewed and, if accepted, will be published in a regular issue of the *Journal of Chemical Information and Modeling*. Once the Virtual Special Issue is complete, all articles will be publicized as a virtual collection, providing additional exposure for the work. We look forward to your contributions.

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

REFERENCES

(1) ChatGPT: five priorities for research. *Nature. 614*: 224−226 (**2023**).
(2) What ChatGPT and generative AI mean for science. *Nature. 614*: 214−216 (**2023**).
(3) Drug discovery companies are customizing ChatGPT: here's how. *Nat. Biotechnol. 41*: 585−586 (**2023**).
(4) ChatGPT for computational materials science: a perspective. *Energy Mater. Adv. 4*: 0026 (**2023**).
(5) Do large language models understand chemistry? A conversation with ChatGPT. *J. Chem. Inf. Model. 63*: 1649−1655 (**2023**).

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