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The Application of Artificial Intelligence in Teaching Practice of the Course Medicinal Chemistry

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Abstract: With the rapid development of artificial intelligence (AI) technologies, the field of education is undergoing profound changes. This paper explores the application of AI in empowering the teaching practice of the course Medicinal Chemistry, a core subject in new engineering programs. Traditional teaching of Medicinal Chemistry faces challenges such as low student motivation, insufficient cultivation of higher-order thinking, and a lack of emotional interaction between teachers and students. This study presents a framework built upon the Superstar Learning platform, utilizing a suite of AI-driven tools to enhance the instructional content and pedagogical methods of this course. By constructing a domain-specific knowledge graph and restructuring the course content, the proposed approach facilitates personalized learning pathways and implements a multifaceted assessment system. These initiatives have significantly improved teaching efficiency and student learning experience, stimulated student interest and innovation, and provided a reference model for AI-empowered education.

Keywords: Medicinal Chemistry; AI; Education; Empowering.

1. Introduction

With the advent of generative artificial intelligence (AI) technologies such as ChatGPT and DeepSeek, AI is driving global transformation at an unprecedented pace, presenting both unprecedented opportunities and challenges across industries. The report of the 20th National Congress of the Communist Party of China explicitly proposed a "trinity" strategic framework integrating education, technology, and talent development [1], positioning educational digital transformation as a crucial mission for building a digital China and a powerful education nation. Driven by dual forces of external technological innovation and evolving talent cultivation demands, the education sector has entered a rapid digital transformation phase, with educational digitization elevated to a national strategic priority.

In February 2022, the 2022 Key Tasks of the Ministry of Education formally outlined the "Education Digitalization Strategy Initiative"[2]. Subsequently, in 2023, the Cyberspace Administration of China, in collaboration with the Ministry of Education and other departments, issued the Interim Measures for the Management of Generative Artificial Intelligence Services, explicitly encouraging innovative applications of generative AI across various industries and domains[3]. Concurrently, six ministries including the Ministry of Science and Technology jointly released guidelines incorporating smart education into the first batch of AI demonstration application scenarios, actively exploring implementations in online classrooms, virtual teaching environments, and smart campus systems.

The emergence of generative AI has not only infused new vitality into education but has significantly accelerated the integration of AI capabilities in teaching, learning, and administrative processes. This technological advancement is driving profound educational reforms characterized by deep convergence between AI and fundamental pedagogical practices as well as management systems.

2. Course Analysis

The Pharmaceutical Engineering is a discipline of engineering that integrates knowledge and skills from multiple disciplines to study and address issues related to processes, engineering, quality, and management in pharmaceutical production[4]. Medicinal Chemistry stands as one of the core courses in this program. Its curriculum encompasses the discovery and invention of new drugs, synthesizing chemical drugs, elucidating the chemical properties of drugs, and investigating the interaction mechanisms between drug molecules and cellular biomacromolecules[5]. As a pioneering field in pharmaceutical sciences, this course serves as a foundational discipline for cultivating students' capabilities in innovative drug research and development[6]. It demands interdisciplinary analytical and integrative skills, combining innovative thinking with professional expertise to equip them with the ability to identify, analyze, and solve complex engineering problems.

However, current Medicinal Chemistry class teaching still faces several pressing issues. From the knowledge acquisition perspective, students generally exhibit a phenomenon of "excessive memorization with limited comprehension," while instructors struggle with "extensive lecturing without in-depth explanation." This results in tedious learning processes, insufficient student motivation, and superficial mastery of key concepts. Regarding competency development, students often encounter difficulties in practical application ("knowing theories but failing to practice"), whereas teaching tends to emphasize "excessive theoretical instruction with limited practical experience" particularly in drug structure-activity relationships (SARs) where fragmented and complex knowledge points create comprehension barriers. Notably, this crucial component serves as the cornerstone for cultivating innovative drug research and development thinking strategies. From the perspective of emotional engagement, there exists "frequent self-study but scarce collaboration" among students, coupled with "unidirectional knowledge delivery with minimal emotional interaction" between teachers and learners. Large class sizes further exacerbate the lack of emotional connectivity and create psychological distance. These challenges collectively indicate that traditional class models are increasingly inadequate in meeting the demands of modern education, necessitating urgent pedagogical innovations to drive transformative changes in teaching methodologies.

The emergence of artificial intelligence (AI) technology has brought new opportunities for transforming the teaching model of Medicinal Chemistry courses. Empowered by AI technology, it can effectively enhance teaching efficiency, optimize teaching content, achieve personalized instruction, and strengthen teacher-student interaction. This, in turn, stimulates students' interest in learning and their innovative abilities, providing strong support for training high-quality talents to meet the future demands of the pharmaceutical field.

3. Practice and Application

3.1. AI-Powered Teaching

3.1.1. Improve the Efficiency of Lesson Preparation

In STEM (Science, Technology, Engineering, and Mathematics) education, long-standing issues persist regarding fixed course knowledge points, outdated teaching materials, antiquated slides, obsolete educational resources, and insufficient integration of course content with current events. To address these challenges, AI technology offers innovative solutions for dynamic teaching resource updates.

In Medicinal Chemistry course, The "Thalidomide Tragedy" (also known as the "Seal Baby" pharmaceutical disaster) serves as a milestone case in medicinal chemistry history, involving chiral drug development and evolving drug regulatory frameworks. Traditional lesson preparation might require teachers to spend hours searching archives, whereas using the WPS Lingxi Large Model, instructors can simply input a structured command like "Introduce the thalidomide drug failure case" to obtain detailed event descriptions and social impact analysis within 30 seconds. The generated content can be directly converted into PPT slides, requiring only minor adjustments before integration into lecture materials or upload to Superstar Learning Platform as extended case studies for autonomous learning.

Similarly, when addressing the ethical controversies surrounding the "Gene-Edited Babies" hot topic, we utilized DeepSeek's multimodal search capabilities to integrate news commentaries, ethics committee statements, and technical schematics within minutes, forming a critical thinking training module. This generative AI-powered teaching resource generation model enables real-time classroom content updates. This approach liberates educators from labor-intensive information gathering, allowing them to focus more energy on instructional design and higher-order thinking guidance.

3.1.2. Restructuring Course Content

The curriculum of "Medicinal Chemistry" is characterized by a large number of diverse knowledge points, loose connections between chapters, and weak logical relationships, particularly in the chemical structures of drugs and structure-activity relationships (SAR), which are key challenges in teaching. In the traditional teaching model, teachers spend extensive time repetitively teaching fundamental knowledge. This approach not only proves pedagogically inefficient for cultivating higher-order cognitive skills, but also engenders tedious learning processes that potentially diminish student engagement. To address these challenges, we have undertaken comprehensive curricular restructuring aligned with the deep integration of artificial intelligence technologies in education. This initiative aims to cultivate students' higher-order abilities and promote a deep transformation of teaching content and models.

In terms of curriculum content, we have reorganized the knowledge system by gradually transferring the instruction of foundational knowledge such as drug classification and structures to students' online autonomous learning. Through the Superstar Learning Platform, we have established a more scientific and efficient learning support system for students. A knowledge graph-centered curriculum framework has been constructed, where the visual presentation of the knowledge graph allows students to clearly discern the logical connections between knowledge points, thereby grasping the structure and context of the course content holistically. The built-in AI teaching assistant feature in the Superstar Learning Platform provides personalized learning path recommendations, real-time learning feedback, and key difficulty analysis based on students' learning progress and knowledge mastery, truly realizing a "student-centered" autonomous learning model. This pedagogical shift from "knowledge transmission" to "competency cultivation" offers robust support for students to adapt to future complex social environments and professional challenges.

3.1.3. Achieve Personalized Education

By leveraging the knowledge graph functionality of the Superstar Learning platform, we have established real-time monitoring of students' knowledge mastery, effectively creating a learning tracking system for each individual. The platform automatically records students' learning trajectories during their interactions, including patterns of rapid concept acquisition and recurring error-prone areas, with all data being systematically captured. The AI teaching assistant analyzes these learning patterns to provide instructors with timely diagnostic feedback, enabling dynamic pedagogical adjustments. When significant difficulties are detected across multiple students regarding particular concepts, instructors can allocate dedicated class time for in-depth explanations or design collaborative learning activities such as group discussions and case studies to enhance comprehension. This AI-powered analytical framework effectively addresses the challenge of monitoring individual learning progress in large-scale classrooms, thereby achieving authentic personalized instruction through data-driven insights.

3.2. AI-Powered Learning

3.2.1. AI Teaching Assistant: Response All the time

The AI teaching assistant on the Superstar Learning platform acts as a constantly available tutor for students, accompanying their learning process all the time. It can rapidly address various questions students encounter during self-study, effectively reducing the difficulty of independent learning. Additionally, based on students' learning progress and needs, it recommends supplementary learning materials, making learning more targeted and greatly improving efficiency. With the AI, students no longer feel helpless when facing problems, which enhances their engagement and enjoyment in learning, allowing each student to steadily progress at their own pace.

3.2.2. Human-Machine Collaboration: Solving Complex Problems

Empowered by AI technology, a profound transformation is occurring in students' learning methods and capability development. With the support of the Learning Pass AI assistant, students can independently master fundamental knowledge, while teachers increasingly serve as classroom facilitators, helping students organize course content and clarify difficult concepts. This division of labor enables students to undertake more challenging higher-order tasks. Through AI-enabled project-based tasks, students can now accomplish more complex and even interdisciplinary assignments, fostering deeper engagement and broader skill development.

In the Medicinal Chemistry course, we have designed three AI-enabled project-based teaching tasks. In the introduction chapter, we designed a research task on "The Application of AI in Drug Development." Students were required to use AI tools to gather information and write a report, clearly distinguishing between the group's perspectives and AI-generated content. The research covered AI's role in drug design, target identification, and drug screening. With AI tools, students efficiently filtered key information and integrated course knowledge to form independent insights. This task enabled students to quickly understand cutting-edge AI applications in pharmacology, grasp the basic processes and strategies of drug development, and foster innovative thinking and research interest.

In the era of artificial intelligence, human-machine collaborative problem-solving has become increasingly prevalent across scientific disciplines. While AI systems demonstrate remarkable efficiency in generating solutions, the epistemic value of these outputs fundamentally depends on the quality of initial problem framing. Therefore, questioning skills, like critical thinking and innovation, are key abilities that students need to cultivate through education. In the homework for the chapter on cholinergic drugs, we asked students to use AI tools to design new cholinergic drugs based on the SAR of cholinergic receptor agonists and to analyze and evaluate their designs. This assignment not only helped students consolidate their understanding of the SAR of cholinergic drugs but also exercised their ability to ask effective questions of AI. Moreover, by analyzing and evaluating AI-generated suggestions, students enhanced their critical thinking. This practical training helped students learn to work with AI, preparing them to solve complex problems in the future.

In the third practice, we tasked students with using AI tools to design a web-based interactive classroom game to identify key medicinal chemistry structures. The game had to cover important chemical structures from the course and enable random student interaction. Previously, such an interdisciplinary task would have been difficult for students without programming knowledge. However, with AI assistance, this complex task became feasible. Students quickly generated game code and optimized the user interface using AI tools. During this process, they not only reinforced their understanding of medicinal chemistry structures but also learned to integrate theoretical knowledge with practical applications. These AI-integrated practical tasks made learning more engaging, sparked students' interest and creativity, and allowed them to expand their computing knowledge and problem-solving skills. Through hands-on practice, students also experienced the immense potential of AI in education.

3.2.3. Innovative Assessment: A Data-Driven Methodology

By utilizing the Superstar Learning Platform, we can comprehensively track and record various aspects of student learning behavior, including classroom participation, homework completion, and quiz scores. This enables a shift from traditional experiential evaluation to data-driven assessment. By providing teachers with detailed records of the learning process, the platform allows for a more objective assessment of student performance. Additionally, it offers students immediate feedback, helping them understand their achievements and areas for improvement. Moreover, by tracking students' learning trajectories, teachers can monitor progress and address issues promptly, leading to timely adjustments in teaching strategies. This transforms evaluation from a diagnostic exercise into a feedback-oriented process, enhancing both teaching and learning.

4. Conclusion

Under the empowerment of AI, the innovative practice of the “Medicinal Chemistry” course has achieved remarkable outcomes. Through the reform of teaching models, expansion of course content, optimization of pedagogical methods, and diversification of learning assessments, the course has not only enhanced teaching efficiency and quality but also significantly stimulated students’ learning motivation and innovative capabilities. This provides strong support for cultivating high-quality pharmaceutical talents equipped to meet future challenges.

Moving forward, we will continue to deepen the application of AI in education. On one hand, we will further optimize course content and teaching methodologies, exploring more interdisciplinary integration points to provide students with richer and cutting-edge learning resources. On the other hand, we will strengthen AI technical training for faculty to enhance their competence in AI-driven instructional design and implementation. Concurrently, we will refine the learning assessment system by leveraging AI technologies to achieve more precise and personalized teaching feedback, thereby better facilitating student growth and development.

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