Integrating AI into education to foster active learning and critical thinking

Reaxys Predictive Retrosynthesis

Case study: Chung Shan Medical University (Taiwan)

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Incorporating the Reaxys Predictive Retrosynthesis AI tool into the curriculum not only trains students to be equipped with synthesis knowledge, but also to prepare them for tackling complex synthesis problems through the development of strong problem-solving skills. AI can expand students' literature readings and enhance their learning experience in ways that make studying more engaging. This approach motivates a new generation of students to become familiar with the AI-assisted research of the future.

The impending influence of AI on educational methodologies is set to reshape student learning. A new generation is embracing the capabilities of generative AI tools to swiftly generate substantial knowledge for diverse tasks. However, discerning the accuracy of AI-provided content remains a pressing challenge. This is a principal reason why traditional learning resources cannot be fully replaced.

In 2023, Elsevier embarked on a mission to engage instructors keen on exploring AI tools within the Reaxys Academic Edition to educational institutions. Our objective was to incorporate next-generation retrosynthetic AI tools into organic chemistry and organic synthesis design courses. This integration aimed to familiarize students with future work dynamics, enabling instructors to infuse innovative AI content into curricula, helping students grasp the benefts from AI tools, and enhancing their proficiency in organic chemistry to help them establish a robust competitive edge for the future.

Integrating Reaxys Predictive Retrosynthesis AI into the classroom: A case study by Professor Chih-Chien Chu, Department of Medical Applied Chemistry, Chung Shan Medical University (Taiwan)

Professor Chih-Chien Chu, Department of Medical Applied Chemistry, Chung Shan Medical University in Taiwan, stands as a fervent advocate of innovation within the realm of education. In 2020, he pioneered augmented reality (AR) teaching aids that brought organic molecules to life, enabling students to "visually" discern the subtle disparities between stereochemical molecules. These innovative teaching aids and teaching methods superseded traditional classroom ones where teachers physically displayed molecular models, alleviating students' cognitive load associated with comprehending abstract spatial concepts. This approach not only facilitated the resolution of intricate stereochemical problems but also kindled students' enthusiasm for learning and empowered them to achieve their learning objectives independently.

In 2023, Professor Chu directed his attention to the organic retrosynthesis course. He reshaped the syllabus for senior students majoring in Chemistry. As a trailblazer in Taiwan, he collaborated with Elsevier in this pedagogical endeavor.

Integrating Reaxys Predictive Retrosynthesis AI tools into his course not only equipped students with the foundational knowledge of classical organic chemistry retrosynthesis, but also cultivated their proficiency in utilizing AI tools to extract crucial information and troubleshoot problems in the future. Professor Chu aptly likens AI to a seasoned laboratory mentor, readily equipping students with a plethora of molecules while offering strategic insights gleaned from pertinent literature. This real-time guidance from the instructor streamlines the process of validating classroom-acquired knowledge for a new generation of students. It fuels their motivation to experiment and propels them toward their research aspirations.

Integrating scenario-based simulation into AI tool learning

Incorporating real-world scenarios, Professor Chu prompts students to immerse themselves as researchers in a pharmaceutical company, simulating the critical drug development journey from conception to synthesis. This approach accommodates diverse levels of comprehension, focus and enthusiasm for organic chemistry among students, making it an effective team effort. Over the initial eight weeks of the course, foundational concepts of organic synthesis reverse engineering are covered using classical retrosynthesis textbooks. Subsequently, students spend four weeks navigating the Reaxys software, engaging in simulations to design novel molecules and conceive artificial synthesis plans. The Reaxys AI tool then enters the picture. The final two to four weeks are devoted to group discussions evaluating the feasibility of the synthesized pathways.

— Professor Chih-Chien Chu
Department of Medical Applied Chemistry,
Chung Shan Medical University (Taiwan)

The journey of molecular design starts with Reaxys. Students delve into published literature to craft novel and unpublished coumarin derivatives. Their exploration begins with tens of thousands of biologically active coumarin derivative structures sourced from the Reaxys database. The emphasis is on specific biological activities, such as anti-cancer or anti-inflammation effects. From this extensive array, students meticulously select potential structures that exhibit interactions with a single biological target protein. Subsequently, these highly active compounds serve as the foundation for students to ideate and create their very own target molecules through brainstorming sessions.

The curriculum then transitions to the central aspect of retrosynthesis planning. Collaboratively, students embark on charting the retrosynthesis pathway for the target molecule, drawing from their textbook knowledge. Following a two-week period, students concurrently analyze the target molecule using Reaxys Predictive Retrosynthesis AI. With the instructor's guidance, students engage in an evaluation of the similarities, distinctions, advantages and constraints inherent in both human-conceived and AI-suggested pathways. These insightful deliberations are then compiled in project reports. Professor Chu's pedagogical strategy encourages students to explore self-designed synthesis paths while also consulting the AI's retrosynthesis predictions. This dual approach stimulates thinking, enhancing student participation and enthusiasm.

Final presentation: Exploring the change and impact of AI integration in the classroom

During the final presentations by students, each group unveils their synthesis strategies crafted through collective brainstorming. Simultaneously, they integrate AI-generated predictions of synthesis pathways. This amalgamation of human ingenuity and AI prompts in-depth discussions on the advantages and disadvantages of each approach, fostering a deep sense of AI tool utilization. These presentations encapsulate students' experiential insights and reflections on their engagement with AI simulation courses. Below, Professor Chu shares his observations and students' feedback:

Figure 1: Student presentations on the use of Reaxys AI

- **Enhanced engagement and enthusiasm:**

  Up to 80% of the four student groups acknowledged heightened interest and motivation in the course. The amalgamation of comprehensive course planning with AI-infused synthesis strategies proved compelling. Students employed their self-designed molecules to reevaluate the solidity of their organic synthesis knowledge. The incorporation of AI-introduced novel reaction pathways, uncharted in textbooks, incited students to delve into pertinent references, ponder AI-guided synthesis feasibility and distinctively incentivized each student. Remarkably, students with laboratory project backgrounds or synthesis experience displayed a profound affinity for the Reaxys AI tool. They adeptly discussed AI pathway merits and optimized synthesis paths using recommended literature. Meanwhile, less experienced peers leveraged AI to enhance their classroom engagement.

- **Seamless AI integration:**

  Every student group was astonished by the user-friendly Reaxys database. The seamless integration of AI and literature allowed them to effortlessly access references throughout data collection, molecular design and even synthetic route planning. Often, the investigation of organic reactions begins with the depiction of organic molecules. However, when faced with unfamiliar molecules that haven't been published, the researcher needs to be adept at the "substructure" search method.

Unfortunately, this approach often consumes time that could be spent delving into essential literature. It's not usually the lack of references that hinders students from finding relevant materials, but rather their inability to draw complex structures. This is where the Reaxys AI technology comes to the rescue, simplifying this intricate and time-intensive task. With a mere sketch of the "target molecule," Reaxys AI can promptly provide literature-backed evidence for each path within ten minutes, liberating students to dedicate their time to comprehending crucial information and engaging in genuinely pivotal learning and exploration.

- **Broadening creative horizons and encouraging innovative thinking through AI:**

  AI ushers in novel perspectives that students may not have contemplated before. One student group recounted an instance in which a Reaxys AI-suggested pathway diverged from conventional thinking by not initiating with coumarin. This departure from the norm took into account cost considerations, challenging the preconceived notion that coumarin derivatives must exclusively originate from coumarin. This scenario underscores how Reaxys AI acts as a catalyst for unexpected insights and creativity, pushing the boundaries of established thought and inspiring innovative perspectives.

The Reaxys AI function has the potential to transcend existing cognitive boundaries. It can aid in formulating efficient synthetic pathways for new compounds, optimize current routes and offer researchers novel insights for crafting synthetic routes.

Quantitative assessment and post-course instructor feedback

Given the varying levels of students in the course, a quantitative post-course survey (Figure 2) reveals students' diverse self-evaluations of their organic chemistry competence before the class, displaying a normal distribution. When it comes to the synthesis path generated through team brainstorming, a level of self-doubt exists (Figure 3). However, responses to the question of whether AI can effectively aid in retrosynthetic design after the course consistently garnered positive ratings of four to five points (with five being the highest score) (Figure 4), signifying a high level of confidence in AI-assisted retrosynthetic pathways (Figure 5). Of notable significance is that upon the exchange of outcomes among groups, none of the groups fully embraced all the paths proposed by AI. Each student expressed varying levels of skepticism regarding the AI-suggested paths, underscoring the indispensable nature of students' critical thinking when reviewing the literature. This highlights the enduring importance of practical hands-on synthesis experience in effective troubleshooting. For organic synthetic chemists, AI functions as an efficient time-saving and idea-generating tool, complementing rather than substituting the roles within the domain of organic synthesis.

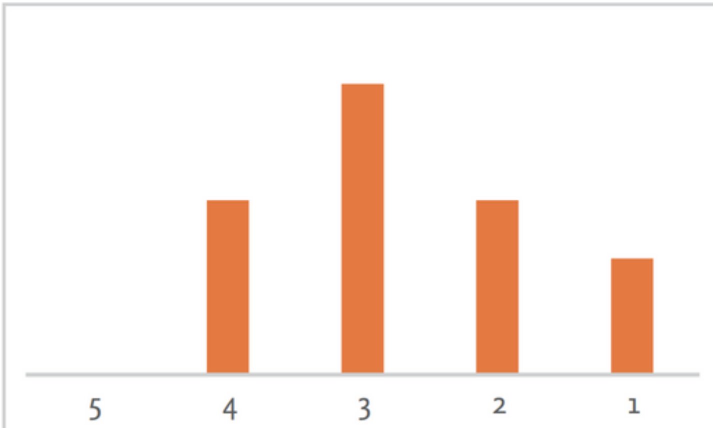

Figure 2: Quantitative Evaluation - Student self-assessment of their organic chemistry pro ciency (with 5 as the highest score and 1 as the lowest).

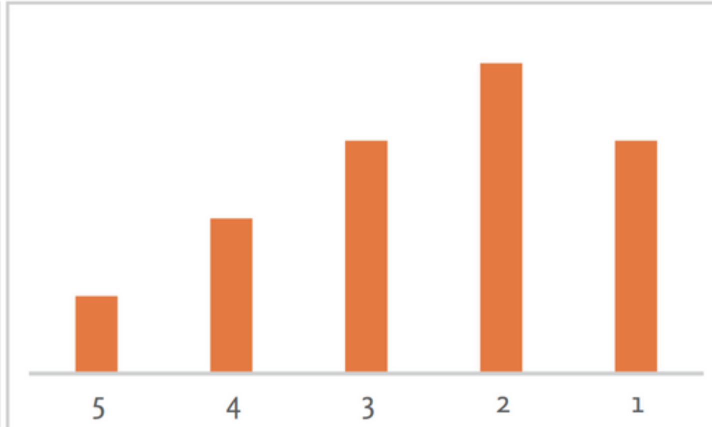

Figure 3: Quantitative Evaluat ion - Student self-assessment of retrosynthetic abilities employing human brain (with 5 as the highest score and 1 as the lowest).

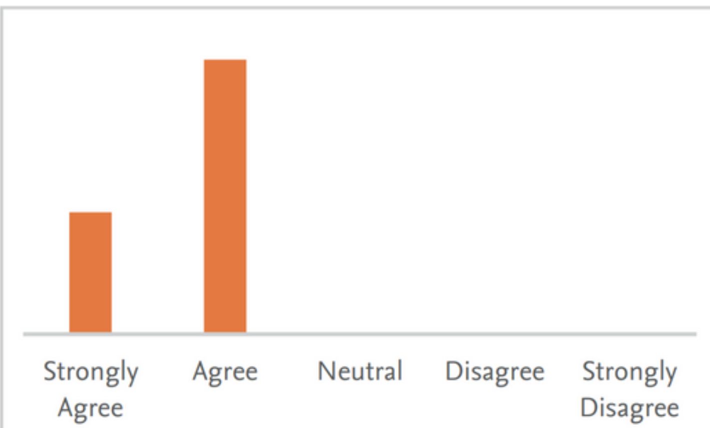

Figure 4: Quantitative Evaluation - Student perceptions regarding the effectiveness of AI in assisting retrosynthetic design.

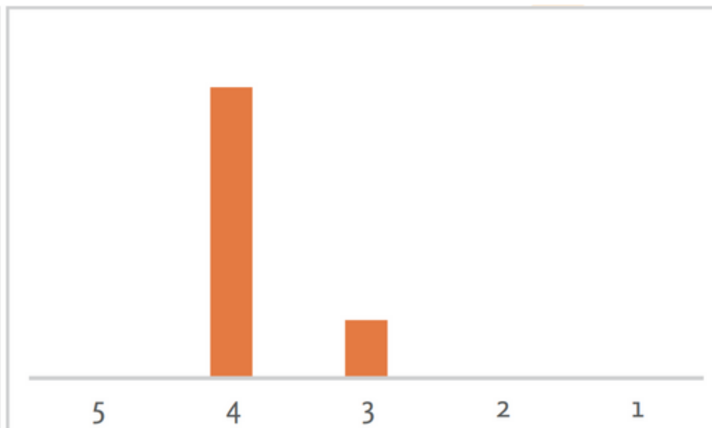

Figure 5: Quantitative Evaluation - Student self-assessment scores for AI-assisted retrosynthesis (with 5 as the highest score and 1 as the lowest.)

Professor Chu offered additional intriguing insights. He noted a significant shift in students' learning dynamics, with increased engagement and intensity. Learning, he observed, transcended the classroom, with students actively seeking appointments with him to discuss the feasibility of identifying alternative paths. Moreover, students displayed heightened awareness of gaps in their knowledge and exhibited meticulousness in report preparation.

His valuable view reflects a positive trend not previously observed in earlier iterations of the course.

Furthermore, Professor Chu shared his perspective on the integration of AI into his curriculum. He likens Reaxys AI to a mentor in a laboratory: a constant companion for offering guidance to students. However, this “senior mentor” not only boasts familiarity with a vast repository of over a thousand books spanning ancient and contemporary knowledge, but also provides access to a comprehensive material library encompassing 15 million responses. This dynamic repository allows for real-time updates of sourcing and pricing information from commercial material base. Consequently, it stands ready to provide invaluable direction and assistance as students grapple with problem-solving, working in tandem with teachers’ guidance. Especially within regional schools, grappling with a scarcity of high-level research personnel such as postdoctoral fellows and doctoral candidates, Reaxys AI offers a potential solution. Additionally, AI tools enable swift generation of teaching plans and enhancement of student interaction. Given that student challenges in synthesis are often multifaceted, transcending mere textbook knowledge, Reaxys AI’s provision of alternative pathways can drive discussions between instructors and students, advancing collaboration and fostering innovative design concepts for synthesis routes.

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