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The Molecular Arena: Gamifying Medicinal Chemistry with HerbaXplorer at SERUMPUN 2026

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On 23rd June 2026, Universiti Teknologi MARA (UiTM), Malaysia, in collaboration with the University of Puthisastra, Cambodia, conducted an interactive Medicinal Chemistry Workshop under the SERUMPUN 2026 programme. The workshop introduced participants to the fundamental concepts of medicinal chemistry, emphasizing the relationship between chemical structure, pharmacological activity, and the therapeutic potential of natural products.

Exploring Drug Discovery Through Interactive Learning

The workshop began with a comprehensive overview of the drug discovery and development process, covering essential concepts including target identification, lead compound optimization, and structure–activity relationships (SAR).

To enhance student engagement and bridge traditional pharmacognosy with digital learning, participants were introduced to HerbaXplorer, an interactive web-based educational platform developed by the NatureRx group under Kumpulan Inovatif dan Kreatif (KIK) at the Faculty of Pharmacy, UiTM. Serving as the official gamification tool for the workshop, HerbaXplorer enabled students to explore medicinal plants and their bioactive compounds through an intuitive and interactive learning environment. Inspired by Hippocrates' famous statement, "Nature itself is the best physician," the activity encouraged students to relate naturally occurring compounds to their potential therapeutic applications.

Figure 1: Demonstration of the HerbaXplorer educational platform by the facilitator during the SERUMPUN 2026 Medicinal Chemistry Workshop.

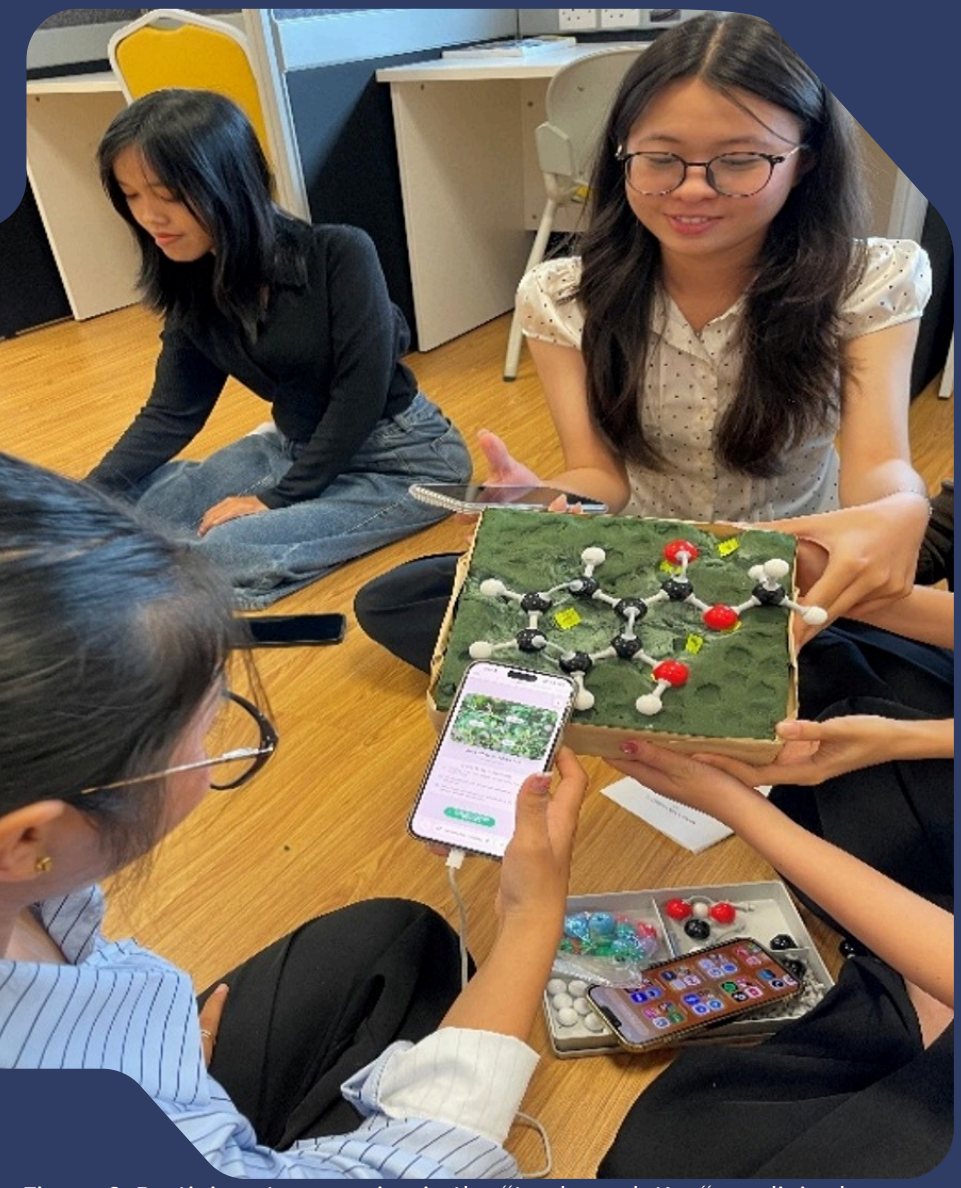

Figure 2. Participants engaging in the “Lock-and-Key“ medicinal chemistry activity using HerbaXplorer.

The theoretical concepts were subsequently reinforced through an interactive “Lock-and-Key“ activity, allowing participants to apply medicinal chemistry principles in a hands-on setting. Acting as medicinal chemists, students used customized sponge models representing three-dimensional protein binding sites together with molecular model kits to construct drug molecules that fit specific biological targets. Using HerbaXplorer on their smartphones, both Malaysian and Cambodian participants explored three-dimensional molecular structures and visualized molecular interactions.

Despite differences in academic backgrounds and language, the application provided a common scientific learning platform, enabling participants to successfully identify, construct, and physically dock representative compounds such as methyl salicylate and nicotine into their respective target sites.

The educational effectiveness of HerbaXplorer was evaluated through a user satisfaction survey. The findings showed that 82% of participants completed compound-search tasks in less than one minute, while 86% agreed that the interactive three-dimensional models improved their understanding of molecular geometry and stereochemistry.

Overall, the workshop successfully combined theoretical knowledge with hands-on learning, demonstrating that HerbaXplorer is an effective and scalable educational platform for enhancing student engagement and understanding of medicinal chemistry.

Figure 3. Participants getting hands-on training by the facilitator in the "Lock-and-Key" medicinal chemistry activity using HerbaXplorer.