

From Molecules to Meaning: **INSIDE THE SUMMER SCHOOL** *2026*

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Can a computer help us understand how molecules interact, predict their behaviour, and provide insights into our research questions?

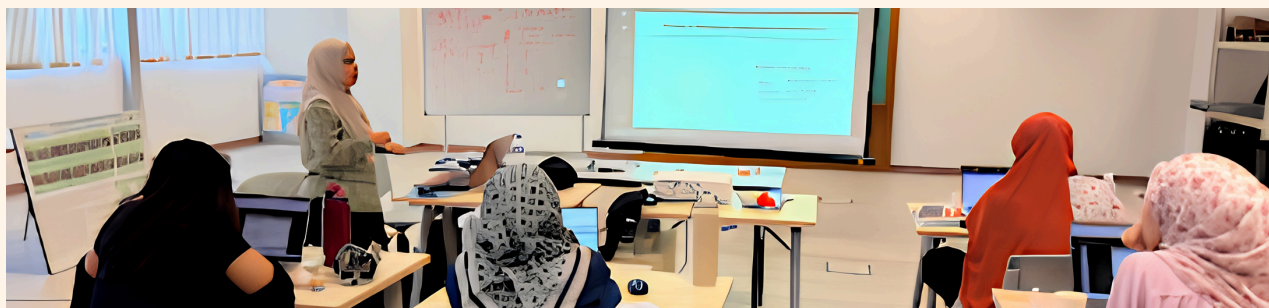
That question captures the journey of the Summer School: Computer-Aided Drug Design (CADD) and Bioinformatics 2026, held from 1 to 4 September 2026 at the Faculty of Pharmacy, UiTM Puncak Alam. Now in its third year, the programme was designed to make computational research more approachable through guided, hands-on learning.



Hands-on, with guidance at every step. Participants worked directly with computational tools, while facilitators provided immediate one-to-one guidance, discussion and troubleshooting throughout the sessions.

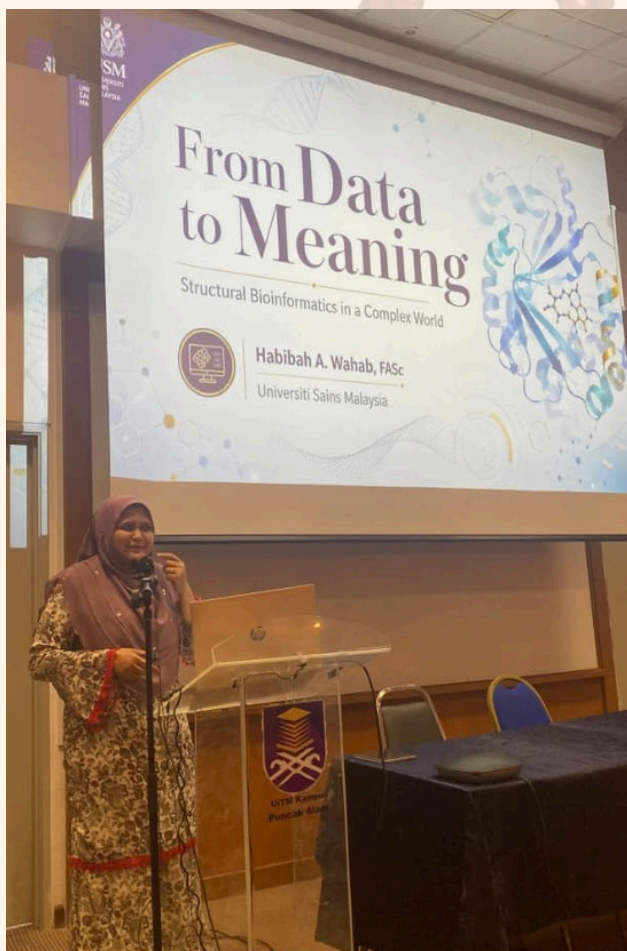
<https://pharmacy.uitm.edu.my>

Across four intensive days, participants progressed from fundamental concepts to increasingly advanced computational workflows. In the CADD and Network Pharmacology track, they explored 3D biomolecular visualisation, sequence analysis, protein modelling, molecular docking, and network pharmacology. The Molecular Dynamics (MD) simulation track introduced participants to the Linux environment and GROMACS before progressing to protein-ligand simulations and advanced MD simulations of lipid bilayers and coarse-grained systems.



Public Talk session

The learning did not stop at the computer screen. A public talk series brought together experts from Universiti Sains Malaysia, Universiti Kebangsaan Malaysia, Universiti Malaya and A*STAR, Singapore. The talks connected participants with wider developments in structural bioinformatics, machine learning, artificial intelligence, precision medicine, and therapeutic discovery.



Summer School 2026 connected participants with leading experts through several public talks, beginning with Distinguished Professor Dr Habibah A. Wahab, Deputy Vice-Chancellor (Research and Innovation), USM, and featuring speakers from UKM, UM and A*STAR Singapore across diverse areas of computational research.

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ore importantly, participants were encouraged to discuss their outputs, troubleshoot challenges and seek immediate one-to-one guidance from facilitators while exploring how these approaches could be applied to their own research. The close interaction throughout the programme also provided opportunities to exchange ideas, build new research connections, and explore future collaborations.

This learning experience was made possible by the collective contributions of our speakers, trainers and facilitators. We sincerely thank Prof. Dr. Habibah A. Wahab, Dr. Lam Su Datt, Prof. Dr. Vannajan Sanghiran Lee, Prof. Dr. Saharuddin Mohamad, Dr. Firdaus Samsudin and Dr. Siti Aisyah Razali for sharing their expertise, and the postgraduate facilitators, Nur Alya Amirah Azhar, Norul Amalina Sabri, Ahmad Merza Mohd Nasir and Syarifuddin Husain, for their dedicated support throughout the programme.

By the end of the four days, computational research was no longer simply something to observe but something participants had experienced, practised, and could begin applying.



Participants and facilitators from the CADD and Network Pharmacology and Molecular Dynamics Simulation tracks, together with invited speakers and the Dean of the Faculty of Pharmacy, UiTM.