MSPP NEWSLETTER

MALAYSIAN SOCIETY OF PHARMACOLOGY AND PHYSIOLOGY (MSPP)

Malaysian Society of Pharmacology and Physiology *November 2025*

MSPP Editorial Message

Dear Esteemed Members of the MSPP,

Warm greetings to all. As we draw closer to the end of 2025, it is truly inspiring to reflect on our collective journey and achievements as a scientific community committed to advancing the frontiers of pharmacology and physiology. This issue of the MSPP Newsletter captures the essence of that shared dedication — to learn, connect, and grow together.

Over the past months, MSPP has continued to champion academic and professional excellence through a series of impactful initiatives. The MSPP Scientific Meeting once again served as a vibrant platform for the exchange of ideas and discovery, complemented by the Travel Grant Award that supported our outstanding members in sharing their work. The Young Investigator Award and Young Teachers Award–Sharing Sessions celebrated the next generation of scholars and educators who embody the future of our disciplines. The MSPP Refresher Course 2025 and our Webinar Series further strengthened pedagogical innovation and collaboration across institutions, while our Bulletin contributions and membership growth continue to reflect the society's expanding reach and engagement.

Looking ahead, MSPP is proud to prepare for our participation in the Federation of the Asian and Oceanian Physiological Societies (FAOPS) meeting — a milestone that reaffirms Malaysia's active presence on the international stage. We eagerly anticipate new opportunities for collaboration, research, and capacity building that will continue to enrich our scientific landscape.

On behalf of the editorial team, I extend my heartfelt appreciation to the MSPP Exco Members, organising committees, collaborating institutions, contributors, and every member and sponsor who has supported our initiatives throughout the year. Your dedication, energy, and passion have been the driving force behind our success.

May this newsletter serve not only as a record of achievements but also as a source of inspiration to continue strengthening our scientific community together, with purpose and unity.

Assoc. Prof. Dr. Noor Azlina Abu Bakar
MSPP Newsletter Editor
noorazlina@unisza.edu.my
Universiti Sultan Zainal Abidin

Contribute to MSPP Newsletter by sending your articles/write-up to: mspp.secretariat@gmail.com

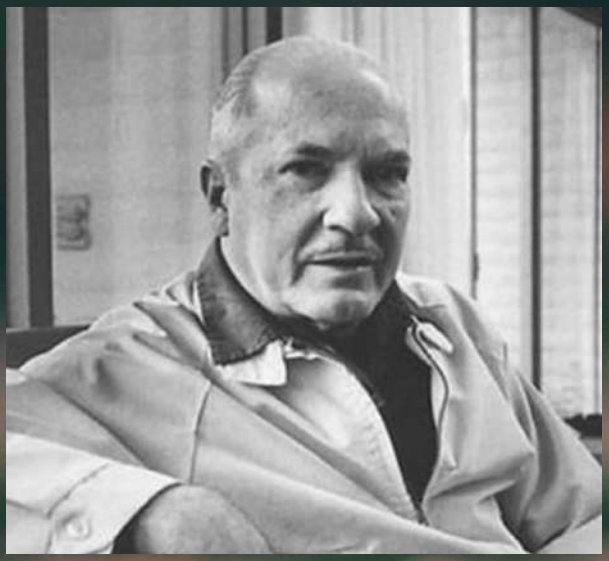
MSPP NEWSLETTER

Malaysian Society of Pharmacology and Physiology *November 2025*

IN THIS ISSUE....

VISIT OUR WEBSITE AND FOLLOW OUR SOCIAL MEDIA

http://www.mspp.com.my/
Malaysian Society of Pharmacology & Physiology
https://www.instagram.com/mspp.secretariat/
https://www.linkedin.com/company/malaysian-society-of-pharmacology-and-physiology/



Everything is theoretically impossible, until it is done

~Robert A. Heinlein~

RESEARCH CORNER

Redefining Drug Discovery through Computational Insight

The Long Road of Traditional Drug Discovery

For decades, discovering a new drug has been a painstaking process. It begins with screening thousands of compounds, followed by cycles of testing, chemical modifications, toxicity evaluation, and multiple trial phases. This journey can take more than a decade, cost billions, and still end in failure when a drug candidate shows poor efficacy or unacceptable side effects. The scale of effort highlights a major challenge in pharmacological research and the need for more predictive approaches to identify promising molecules early on.

Bioinformatics: Redefining the Discovery Pipeline

Bioinformatics has revolutionised drug discovery by allowing researchers to predict drug–target interactions before experimental testing. Methods such as molecular docking, molecular dynamics, and cheminformatics enable rapid in silico screening of extensive chemical libraries, pinpointing compounds with strong predicted binding affinities and favourable pharmacological profiles.

From Simulation to Success: The Case of Imatinib

Molecular docking predicts how a small molecule binds to a protein's active or binding site, helping to estimate the strength and orientation of the interaction, while molecular dynamics tests the stability of this interaction under physiological conditions. Together, these methods offer deeper insight into the behaviour and stability of drug candidates within biological systems.

The impact of this computational approach is well illustrated in successful drug discovery efforts. It reduces time, cost, and experimental redundancy, increasing the chances of success in later development stages.

A notable example is the development of imatinib (Gleevec) for chronic myeloid leukaemia (CML). Genomic studies first identified the BCR-ABL fusion gene that produces the oncogenic tyrosine kinase driving CML. Molecular docking was then used to virtually screen compounds, and molecular dynamics simulations verified the binding of imatinib, guiding the design of this highly selective kinase inhibitor that transformed CML treatment from chemotherapy to targeted therapy (Jørgensen, 2019; Konda et al., 2023).

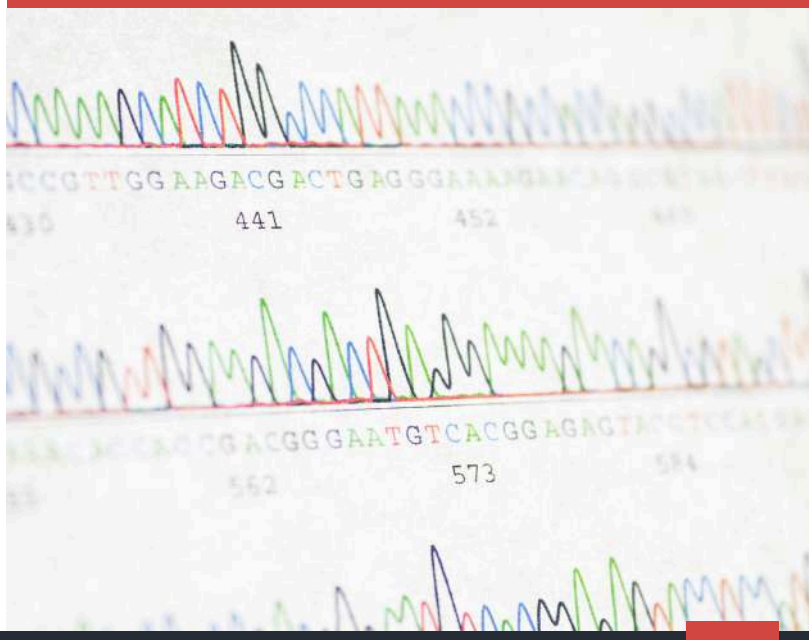
Drug Repurposing and New Therapeutic Indications

Beyond de novo drug discovery, bioinformatics significantly accelerates the repurposing of existing drugs for new therapeutic uses. Paclitaxel, a chemotherapy drug derived from the bark of the Pacific yew tree (Taxus brevifolia), was first approved for ovarian cancer and was later redesigned through computational modelling. Docking studies and pharmacokinetic profiling led to the formulation of a safer, more effective albumin-bound form, Nab-paclitaxel (Abraxane), now also approved by the United States Food and Drug Administration (US FDA) for breast and lung cancers (Chaurasia et al., 2023; Mangilit et al., 2024; Paal et al., 2007; Sati et al., 2024; Suwannasom et al., 2023).

A Turning Point: Bioinformatics and COVID-19 Drug Discovery

The urgency of the COVID-19 outbreak accelerated the use of bioinformatics in antiviral drug discovery. Computational techniques like virtual screening modelled key viral components for SARS-CoV-2 replication, such as the RNA-dependent RNA polymerase (RdRp) and the main protease (Mpro) (Balkrishna et al., 2021; Piplani et al., 2022). Early research using computational tools showed the strong binding of remdesivir to the RdRP target (Elfiky, 2020), guided the clinical fast-tracking and subsequent designation of remdesivir (Veklury) as the first fully US FDA-approved COVID-19 antiviral in October 2020 (U.S. Food and Drug Administration, 2020).

On the other hand, the Mpro target was subjected to rational drug design, guiding the development of nirmatrelvir, a highly specific Mpro inhibitor, combined with the CYP3A inhibitor ritonavir to form Paxlovid (Owen et al., 2021). The resulting development speed led to receiving Emergency Use Authorisation (EUA) in December 2021 (U.S. Food and Drug Administration, 2021), fundamentally validating computational methods as a high-speed pipeline for critical drug development. More recent approaches, combining molecular docking with artificial intelligence, have identified additional candidates, such as paritaprevir and vinblastine derivatives, demonstrating how computational insights can guide real-world drug repurposing (Aqeel et al., 2025; Negru et al., 2022).



The Future: Smarter, Faster, More Predictive

The integration of bioinformatics has turned drug discovery into a more innovative science, driven by prediction rather than trial and error. For pharmacologists, it represents a shift towards data-guided precision, bridging the gap between molecular understanding and therapeutic success.

With each new algorithm and simulation, bioinformatics continues to shorten the path from molecule to medicine, reshaping the future of pharmacological research. For today's pharmacologists, bioinformatics represents more than a tool; it is a catalyst, turning discovery into design and bringing tomorrow's medicines closer to reality.

By : Assoc. Prof. Ts. Dr. Azlini Binti Ismail
dr_azlini@iium.edu.my
Kulliyyah of Dentistry,
International Islamic University Malaysia

References:

- Aqeel, I., Majid, A., Albanyan, A., & Wasfi, H. (2025). Drug repurposing targeting COVID-19 3CL protease using molecular docking and machine learning regression approaches. Scientific Reports, 15(1), 18722. https://doi.org/10.1038/s41598-025-02773-7
- Balkrishna, A., Mittal, R., Sharma, G., & Arya, V. (2021). Computational insights of phytochemical-driven disruption of RNA-dependent RNA polymerase-mediated replication of coronavirus: a strategic treatment plan against coronavirus disease 2019. New Microbes and New Infections, 41, 100878. https://doi.org/10.1016/j.nmni.2021.100878
- Chaurasia, M., Singh, R., Sur, S., & Flora, S. (2023). A review of FDA approved drugs and their formulations for the treatment of breast cancer. Frontiers in Pharmacology, 14, 1184472.

- Aqeel, I., Majid, A., Albanyan, A., & Wasfi, H. (2025). Drug repurposing targeting COVID-19 3CL protease using molecular docking and machine learning regression approaches. Scientific Reports, 15(1), 18722. https://doi.org/10.1038/s41598-025-02773-7
- Balkrishna, A., Mittal, R., Sharma, G., & Arya, V. (2021). Computational insights of phytochemical-driven disruption of RNA-dependent RNA polymerase-mediated replication of coronavirus: a strategic treatment plan against coronavirus disease 2019. New Microbes and New Infections, 41, 100878. https://doi.org/10.1016/j.nmni.2021.100878
- Chaurasia, M., Singh, R., Sur, S., & Flora, S. (2023). A review of FDA approved drugs and their formulations for the treatment of breast cancer. Frontiers in Pharmacology, 14, 1184472.

- Elfiky, A. A. (2020). Anti-HCV, nucleotide inhibitors, repurposing against COVID-19. Life Sciences, 248, 117477. https://doi.org/10.1016/j.lfs.2020.117477
- Jørgensen, J. T. (2019). Twenty Years with personalized medicine: past, present, and future of individualized pharmacotherapy. Oncologist, 24(7), e432-e440. https://doi.org/10.1634/theoncologist.2019-0054
- Konda, P., Garinet, S., Van Allen, E. M., & Viswanathan, S. R. (2023). Genome-guided discovery of cancer therapeutic targets. Cell Reports, 42(8), 112978. https://doi.org/10.1016/j.celrep.2023.112978
- Mangilit, N. J. D., Arkoncel, A. B. S., Baylon, K. M. D., Eslabra, J. M. V., De Borja, J. L. D., Nakama, J. G., Esmalla, M. S. A., Labrador, A. M., Paulin, J. P., & Santiago-Bautista, M. R. (2024). Molecular docking and pharmacokinetic profiling of nab-paclitaxel as advanced chemotherapeutic agent against HER-2 positive breast cancer patients. Asian Pacific Journal of Cancer Prevention, 25(10), 3447. https://doi.org/10.31557/APJCP.2024.25.10.3447
- Negru, P. A., Miculas, D. C., Behl, T., Bungau, A. F., Marin, R. C., & Bungau, S. G. (2022). Virtual screening of substances used in the treatment of SARS-CoV-2 infection and analysis of compounds with known action on structurally similar proteins from other viruses. Biomedicine & Pharmacotherapy, 153, 113432. https://doi.org/10.1016/j.biopha.2022.113432
- Owen, D. R., Allerton, C. M. N., Anderson, A. S., Aschenbrenner, L., Avery, M., Berritt, S., Boras, B., Cardin, R. D., Carlo, A., Coffman, K. J., Dantonio, A., Di, L., Eng, H., Ferre, R., Gajiwala, K. S., Gibson, S. A., Greasley, S. E., Hurst, B. L., Kadar, E. P., Kalgutkar, A. S., Lee, J. C., Lee, J., Liu, W., Mason, S. W., Noell, S., Novak, J. J., Obach, R. S., Ogilvie, K., Patel, N. C., Pettersson, M., Rai, D. K., Reese, M. R., Sammons, M. F., Sathish, J. G., Singh, R. S. P., Steppan, C. M., Stewart, A. E., Tuttle, J. B., Updyke, L., Verhoest, P. R., Wei, L., Yang, Q., & Zhu, Y. (2021). An oral SARS-CoV-2 Mpro inhibitor clinical candidate for the treatment of COVID-19. Science, 374(6575), 1586-1593. https://doi.org/10.1126/science.abl4784
- Paal, K., Shkarupin, A., & Beckford, L. (2007). Paclitaxel binding to human serum albumin—Automated docking studies. Bioorganic & Medicinal Chemistry, 15(3), 1323-1329. https://doi.org/10.1016/j.bmc.2006.11.012
- Piplani, S., Singh, P., Petrovsky, N., & Winkler, D. A. (2022). Computational repurposing of drugs and natural products against SARS-CoV-2 Main Protease (Mpro) as potential COVID-19 therapies. Frontiers in Molecular Biosciences,9-2022. https://doi.org/10.3389/fmolb.2022.781039
- Sati, P., Sharma, E., Dhyani, P., Attri, D. C., Rana, R., Kiyekbayeva, L., Büsselberg, D., Samuel, S. M., & Sharifi-Rad, J. (2024). Paclitaxel and its semi-synthetic derivatives: comprehensive insights into chemical structure, mechanisms of action, and anticancer properties. European Journal of Medical Research, 29(1), 90. https://doi.org/10.1186/s40001-024-01657-2
- Suwannasom, N., Sriaksorn, N., Thepmalee, C., Thephinlap, C., Tanamatayarat, P., Khoothiam, K., Bäuemler, H., & Na-Ek, N. (2023). Efficacy and safety of nanoparticle albumin-bound paclitaxel in advanced non-small cell lung cancer: a systematic review and meta-analysis of clinical trials and observational studies. Heliyon, 9(11), e21903. https://doi.org/10.1016/j.heliyon.2023.e21903
- U.S. Food and Drug Administration. (2020, October 22). FDA Approves First Treatment for COVID-19. [Press Release]. Retrieved from: https://www.fda.gov/news-events/press-announcements/fda-approves-first-treatment-covid-19
- U.S. Food and Drug Administration. (2021, December 22). FDA Authorizes First Oral Antiviral for Treatment of COVID-19. [Press Release]. Retrieved from: https://www.fda.gov/news-events/press-announcements/fda-authorizes-first-oral-antiviral-treatment-covid-19