



Current Trends in Medicinal Chemistry and Its Future

Medicinal chemistry is a multidisciplinary area in chemistry that connects chemistry, applied chemistry, pharmacy, and relevant areas. It also directed to discovery, development, and refinement of therapies for plants and animals. In modern science, it is presently a fast and demanding interdisciplinary research area (Patrick, 2023). It mainly aims to improve our lives through synthesizing, characterizing, and developing new drugs as well as modifying existing bioactive moieties to combat various diseases and disorders (Toenjes & Gustafson, 2018).

In general, medicinal chemistry discusses the design, chemical synthesis, and development of new formulations with the help of organic chemistry, pharmacology, and biological perspectives. Traditionally, medicinal chemistry started its journey from plant products to manage various ailments in humans. Sumerian civilization used hundreds of medicinal plants (over 250 plants), including opium on clay tablets in 3000 BC (around 5000 years ago). Many records have been identified in Babylon, Egypt, China, ancient Greece, Rome, and India about the use of medicinal plants and their derivatives in human diseases. Hippocrates and Galen also described the therapeutic value of plants (Jampilek, 2019; Patrick, 2023). However, the information regarding the usage of plants was gathered into 'Materia Medica' and pharmacopoeias during the Middle Ages. The seventeenth and eighteenth centuries are the golden age for the discovery of several useful medicinal plants (Farrant, 2020). Salicylic acid, discovered from willow bark in 1870 with an analgesic effect, was a breakthrough in medicinal chemistry. Currently, we have more than 120 important drugs that are derived from medicinal plants and are used worldwide. And now our medical library is rich with thousands of bioactive compounds.

Lipinski's rule of five (Pfizer's rule of five, rule of thumb, or the rule of five (RO5)) evaluates drug likeness based on the observation that most orally administered drugs are relatively small and moderately lipophilic molecules. This rule describes molecular properties important for a drug's ADME (absorption, distribution, metabolism, and excretion) in a human body (Lipinski, 2016). In the past, synthesis and modifications of bioactive compounds as well as small molecular weight compounds were highly discussed. However, in the modern era, there is more concern about simpler-to-assemble, higher molecular weight compounds and targeted degradation derivatives, which are of great interest, which is pushing us to think about the fate of RO5 in the near future (Eyube, 2024).

Modern medicinal chemistry believes that a specific disease needs a specific treatment (Eyube, 2024). Although viral infections are yet to be managed with targeted molecules, which we normally rely on preventive vaccinations for, many bacterial infection cases have been solved by current antibiotic therapies. To date, various

strategies have been followed in the case of cancer, metabolic and neurological diseases and disorders, and so on. Simpler-to-assemble, higher molecular weight compounds, such as PROteolysis Targeting Chimeras (PROTACs), have been identified as promising candidates in cancer, infectious diseases, etc. (Zhao et al., 2023). Another practical example is antisense oligonucleotides that are increasing interest for the treatment of infectious diseases (Watts, 2018).

Nano-based drug synthesis and utilization is another interesting sector of modern medicinal chemistry (Mattioli et al., 2024). On the other hand, pro-drug development, modulator synthesis, enzymatic preparation, targeting protein-protein druggable cavities, and so on are some other important strategies of modern medicinal chemistry (Vanden Eynde et al., 2019). Modern medicinal chemistry has an advanced focus on solubility modification, bioavailability enhancement, and toxicity management in the host.

One potential limitation for the medicinal chemistry has been identified since its starting point is the slowest process to discover a new drug candidate (Partridge et al., 2020). However, combinatorial synthesis and diversity-oriented synthesis are known key technologies to solve this issue (Kennedy et al., 2008; Collins et al., 2016). Therefore, the generation of structurally diverse hit compounds is possible in a short period of time for the biological assays. Moreover, virtual screening, either structure-, ligand-, or fragment-based techniques, has been discovered as some potential new ways for the discovery of new active molecules (Zhou et al., 2021). Additionally, activity-directed synthesis is another emerging approach that allows crude reaction mixtures to be directly screened for checking biological activity (Karageorgis et al., 2020). Therefore, current approaches in medicinal chemistry are not centered on the generation of academic knowledge; their consequential approaches and advantages are also directed towards the industrial production of new therapeutic molecules.

The COVID-19 situation also proves that medicinal scientists played pivotal roles through collaboration and sharing research data (Ghosh et al., 2020); is it possible to handle the upcoming challenges? In short, medicinal chemistry is a multidisciplinary subject that accommodates knowledge, skills, techniques, and approaches with advanced technologies to do for the human beings and other animals and resolve existing and upcoming challenges worldwide.

Editorial Note

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Conflict of Interest

The author declared that they have no conflict of interest.



References

- Collins, S., Bartlett, S., Nie, F., Sore, H. F., & Spring, D. R. (2016). Diversity-oriented synthesis of macrocycle libraries for drug discovery and chemical biology. *Synthesis*, 48(10), 1457-1473.
- Eyube, M. (2024). Medicinal Chemistry: Scope, Applications, and Significance in Modern Science. *International Journal of Innovative Research in Computer Science & Technology*, 9(1).
- Farrant, E. (2020). Automation of synthesis in medicinal chemistry: Progress and challenges. *ACS Medicinal Chemistry Letters*, 11(8), 1506-1513.
- Ghosh, A. K., Brindisi, M., Shahabi, D., Chapman, M. E., & Mesecar, A. D. (2020). Drug development and medicinal chemistry efforts toward SARS-coronavirus and Covid-19 therapeutics. *ChemMedChem*, 15(11), 907-932.
- Jampilek, J. (2019). Heterocycles in medicinal chemistry. *Molecules*, 24(21), 3839.
- Karageorgis, G., Liver, S., & Nelson, A. (2020). Activity-Directed Synthesis: A Flexible Approach for Lead Generation. *ChemMedChem*, 15(19), 1776-1782.
- Kennedy, J. P., Williams, L., Bridges, T. M., Daniels, R. N., Weaver, D., & Lindsley, C. W. (2008). Application of combinatorial chemistry science on modern drug discovery. *Journal of combinatorial chemistry*, 10(3), 345-354.
- Lipinski, C. A. (2016). Rule of five in 2015 and beyond: Target and ligand structural limitations, ligand chemistry structure and drug discovery project decisions. *Advanced drug delivery reviews*, 101, 34-41.
- Mattioli, E. J., Cipriani, B., Zerbetto, F., Marforio, T. D., & Calvaresi, M. (2024). Interaction of Au (iii) with amino acids: a vade mecum for medicinal chemistry and nanotechnology. *Journal of Materials Chemistry B*, 12(21), 5162-5170.
- Partridge, L., Fuentealba, M., & Kennedy, B. K. (2020). The quest to slow ageing through drug discovery. *Nature Reviews Drug Discovery*, 19(8), 513-532.
- Patrick, G. L. (2023). *An introduction to medicinal chemistry*. Oxford university press.
- Toenjes, S. T., & Gustafson, J. L. (2018). Atropisomerism in medicinal chemistry: challenges and opportunities. *Future medicinal chemistry*, 10(4), 409-422.
- Vanden Eynde, J. J., Mangoni, A. A., Rautio, J., Leprince, J., Azuma, Y. T., García-Sosa, A. T., Hulme, C., Jampilek, J., Karaman, R., Li, W., Gomes, P. A. C., Hadjipavlou-Litina, D., Capasso, R., Geronikaki, A., Cerchia, L., Sabatier, J. M., Ragno, R., Tuccinardi, T., Trabocchi, A., Winum, J. Y., ... Muñoz-Torrero, D. (2019). Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes-6. *Molecules (Basel, Switzerland)*, 25(1), 119. <https://doi.org/10.3390/molecules25010119>
- Watts, J. K. (2018). The medicinal chemistry of antisense oligonucleotides. *Oligonucleotide-Based Drugs and Therapeutics: Preclinical and Clinical Considerations for Development*, 39-90.
- Zhao, X., Chen, Y., Su, H., & Zhang, L. (2023). From classic medicinal chemistry to state-of-the-art interdisciplinary medicine: Recent advances in proteolysis-targeting chimeras technology. *Interdisciplinary Medicine*, 1(2), e20230004.
- Zhou, H., Cao, H., & Skolnick, J. (2021). FRAGSITE: a fragment-based approach for virtual ligand screening. *Journal of chemical information and modeling*, 61(4), 2074-2089.

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