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Editorial

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Click-based and Computer-assisted Modern Chemistry Insights and Discoveries

Nature-based drug discovery, design, and development is a popular approach since the nineteenth century. To date, we have around 40% pharmaceutical drugs of both natural origins and their semi-synthetic derivatives. Undoubtedly, nature-origin drug discovery and development constitutes one of the major platforms in medicinal chemistry. However, the traditional approaches are getting old day by day in the context of the outcome, merits, and applicability of the above-mentioned 4D process (Islam, 2025). Therefore, the modern researchers are always in search of new, time- and cost-effective, but sensitive and outcome-based strategies in medicinal chemistry and drug discovery.

Discovery, design, and development of drugs from natural origins are always expensive and time-demanding processes. It is because each step has a high failure rate. The modern medicinal scientists realize the fact, and they are continuously searching for new and rapid strategies to overcome the limitations and challenges integrated into the overall process. The click chemistry (CC) and computer-assisted drug design (CADD) are two modern, hopeful, and equally popular approaches in drug development research. CC permits a promising chemo-selective synthetic process; therefore, molecular coupling has been possible for fragments since 2001 (Zhang et al., 2021; Ashe, 2022). This process allows effective synthesis and modification of new drug candidates from a variety of sources with advanced target delivery, while CADD is helpful for the target identification, search and optimization of lead compounds, prediction of pharmacokinetic and pharmacodynamic parameters, and so on. The CADD-based study emerged in the 1970s. There is no doubt that CADD has already attracted modern drug scientists due to its potential for the acceleration and reduction of time and cost of the drug development process (Wu et al., 2020).

Patent restrictions are one of the major obstacles in the drug development process. The CC is considered a magic weapon for the researchers to overcome this obstacle through its magic, as it can transform the active compound skeleton rapidly and improve the activity of drug candidates (Mironov et al., 2023). The CC is able to synthesize and modify natural products, adjust certain chain lengths, and improve the targeting capacity of the drug molecules (Spieler et al., 2020; Brauer et al., 2022). It is to be noted that many existing drugs have some shortcomings, including poor selectivity and stability in the host, extensive synthetic routes, side effects, and so on. The CC is a promising solution for these cases (Ali et al., 2022).

On the other hand, CADD is already evident to employ for effective and efficient designing and development of new drugs. Silicon-chip-based methods are frequently used for the identification of targets, seeking out and optimization of lead compounds, and prediction of all possible biopharmaceutical properties, which is one of the potential weapons of the researchers to understand possible beneficial and harmful effects of a drug candidate in the host. Molecular docking and dynamics, virtual screening, along with the pharmacophore and ADMET (absorption, distribution, metabolism, excretion, and toxicity) prediction, are some popularly known approaches in CADD study (Wadanambiet al., 2023).

Besides time, cost, and efforts, both CC and CADD approaches are considered readily updatable methods, which is a denominator for taking upcoming challenges and overcoming problems in discovery, designing, and developing therapeutic moieties from a variety of sources. Another important fact is to reserve plant and animal kingdoms' rights in the universe.

Editorial Note

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Conflict of interest

None to declare.

References

Ali, I., Gulfam, M., Jo, S. H., Seo, J.W., Rizwan, A., Park, S. H., et al. (2022). Reductionresponsive and bioorthogonal carboxymethyl cellulose based soft hydrogels cross-linked via IEDDA click chemistry for cancer therapy application. *International Journal of Biological Macromolecules 219*, 109–120. https://doi.org/10.1016/j.ijbiomac.2022.07.229

Ashe, K. (2022). Chemistry just a click away. *Nature Chemistry 14* (56), 1341. https://doi.org/10.1038/s41557-022-01108-7

Brauer, J., Mötzing, M., Gröst, C., Hoffmann, R., and Berg, T. (2022). Templated generation of a bcl-xL inhibitor by isomer-free SPAAC based on azacyclonon-5-yne. *Chemistry 28* (66), e202202259. https://doi.org/10.1002/chem.202202259

Islam, M. T. (2025). Current trends in medicinal chemistry and its future. *Journal of Medicinal Chemistry and Therapeutics 1*(5): 5-2. https://doi.org/10.71193/jmct.20250003

Mironov, M. E., Rybalova, T. V., Pokrovskii, M. A., Emaminia, F., Gandalipov, E. R., Pokrovskii, A. J., et al. (2023). Synthesis of fully functionalized spirostanic 1,2,3-triazoles by the three component reaction of diosgenin azides with acetophenones and aryl aldehydes and their biological evaluation as antiproliferative agents. *Steroids 190*, 109133. https://doi.org/10.1016/j.steroids.2022.109133

Spieler, V., Ludwig, M. G., Dawson, J., Tigani, B., Littlewood-Evans, A., Safina, C., et al. (2020). Targeting interleukin-4 to the arthritic joint. *Journal of Control Release 326*, 172–180. https://doi.org/10.1016/j.jconrel.2020.07.005

Wadanambi, P. M., Jayathilaka, N., and Seneviratne, K. N. (2023). A computational study of carbazole alkaloids from Murraya koenigii as potential SARS-CoV-2 main protease inhibitors. *Applied Biochemistry and Biotechnology 195*(1), 573–596. https://doi.org/10.1007/s12010-022-04138-6

https://doi.org/10.71193/jcid.20250003

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Wu, F., Zhou, Y., Li, L., Shen, X., Chen, G., Wang, X., et al. (2020). Computational approaches in preclinical studies on drug discovery and development. *Frontiers in Chemistry 4*, 726. https://doi.org/10.3389/fchem.2020.00726

Zhang, X., Zhang, S., Zhao, S., Wang, X., Liu, B., and Xu, H. (2021). Click chemistry in natural product modification. *Frontiers in Chemistry 5*, 774977. https://doi.org/10.3389/fchem.2021.774977

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