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Automated Technologies for Medicinal Chemistry

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Introduction

Drug discovery is an ongoing process that has always been driven by the urge to provide novel therapies to patients as soon as feasible. This chapter will examine the history of medicinal chemistry, how it has evolved over time as a result of the development of new enabling technologies, and how early developments in synthesis, purification, and analysis have laid the groundwork for the development of the current automated and enabling technologies. This chapter will address upcoming technologies in addition to those that are now well-established, as well as how they will affect drug discovery in the future and the function of medicinal chemists.

In order to find safe and effective medications, medicinal chemistry plays a vital and underpinning role in chemical biology, pharmacology, and medicine. Targeting the purpose of producing new chemical probes and lead compounds for novel and druggable targets, small molecule medicinal chemistry relies on iterative learning cycles made up of compound design, synthesis, testing, and data analysis. Traditional methods can take a long time from hypothesis to results, which reduces the number of molecules that can move into clinical research. With the use of enabling technologies, which have significant promise for enhancing the drug discovery process, this problem can be solved [1].

Description

Since the 1990s genomics craze, scientists have tried to use automation to speed up their studies. Automation had been successfully used in other areas, such as industrial environments, where basically identical operations were carried out on largely identical products. This method could be used in research for both routine operations like handling liquids and for more analytical work like setting up and analysing biochemical assay plates. It was also successfully used in processes like PCR, where the same procedure was repeatedly carried out on basically the same things (with there being only four monomers in DNA synthesis) [2].

Peptide solid phase synthesis provides another early example of successful automation in synthesis. Almost as soon as Merrifield1 developed polystyrene supported peptide synthesis in the 1960s, automated synthesisers were created, and these have since been improved to provide effective access to peptides. Without a question, peptide synthesis has been a success for automation. This is related to two significant elements.

Researchers have noted that the use of the more kit-ized chemistries can result in a lack of structural diversity, despite the fact that these innovations have been successful in significantly increasing the efficiency of some tasks, such as the creation of small targeted libraries for early stage hit and lead optimization. Five years and two distinct approaches later, both groups found a substantial trend in the kinds of processes used to access molecules in medicinal chemistry programmes. A clear preference was shown for parallel chemistry-capable processes, such as the Suzuki-Mayura coupling of carbon to generate carbon-carbon bonds and the production of amide bonds [3].

Additionally, proprietary platforms have been created in industrial laboratories. Despite frequently utilising more advanced automation and synthesis techniques (such as new chemistries or flow chemistry systems), these platforms still depend on batching comparable operations. To shorten cycle times, several researchers have also concentrated on integrating synthesis with other laboratory procedures like analysis, purification, and screening.

The cartridge-based system created by Synple32, for which reagent kits can be ordered in cartridge format for typical reactions, is another illustration of kit chemistry. The technique uses solid supported scavengers to automatically complete the work up once the reaction takes place in a vial. The cartridges' current focus is restricted to the reactions of importance to chemical biologists, such as protac and biotinylation, as well as the Mitsunobu reaction, reductive amination, and heterocycle synthesis.

With the lack of reproducibility in the scientific literature being increasingly highlighted as a resource waster in both the originator groups and those that attempt to repeat or expand on the research, synthesis automation has always held out the promise of increased productivity and improved reproducibility. However, the promise has not been kept in terms of implementation.

The use of automated systems to perform synthetic chemistry in order to acquire more information about the processes and results has also been a theme. This could be a crucial strategy for enhancing the reproducibility and repeatability of synthesis, albeit being in its early phases. Additionally, improvements in computing power seem to be making synthesis planning tools more beneficial, since they now seem to be providing a viable option for automated idea generation for route planning and even the generation of novel chemical step ideas. Although AI will undoubtedly help with the work of coming up with synthesis ideas, this does not now represent a bottleneck in many respects. Though sluggish and rate limiting, practical experimentation is nonetheless necessary to test synthesis theories [4,5].

Conclusion

Structure-activity relationships (SAR) are defined iteratively in medicinal chemistry through computational design, compound synthesis, biological tests, and data gathering. Analysis of the collected data informs the next cycle of learning. Typically, cycle stages are compartmentalised, there are few substances available for clinical trials, delayed explorations, and compounding delays between hypotheses and outcomes. Therefore, methods that facilitate activities within a single compartment while integrating the many disciplines are extremely desirable.Medicinal chemistry, an interdisciplinary field of study that sits at the intersection of chemical biology, pharmacology, and medicine. Discovering chemical probes and lead compounds for unexplored biological targets, proving the drug ability of the target, and addressing problems that affect drug efficacy and failure are the three major goals of medicinal chemistry. Most crucially, medicinal chemistry makes it possible to identify clinical candidates and offers cutting-edge methods for enhancing the scope and calibre of hit- and lead-finding phases, which, though sometimes disregarded, are essential to lowering attrition in drug development.

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Conflict of Interest

There are no conflicts of interest by author.

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