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Basic idea of combinatorial chemistry

Sudha M*

Vivekavardhini College, Kothagudem, Telangana, India

***Corresponding author:** Sudha M, MSc Organic Chemistry, Vivekavardhini College, Kothagudem, Telangana, India, E-mail: sudhamantri29@gmail.com

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Abstract

This branch of chemistry is extremely young, but during this short time it's had profound effects. This will be seen by its impact on medicinal chemistry and, especially, the drug design process. Traditionally, potential lead compounds were synthesized one at a time. The biological activity of this compound was assayed, and therefore the results would be reflected within the next round of design. This traditional method was useful, but time consuming and expensive. Computational chemistry led to more rational design of compounds to be tested, and high throughput screening led to quick in vitro assays. Synthesis of one compound at a time could not continue, and thus became the speed limiting step within the process. Combinatorial chemistry was the answer to the present problem.

Size: depends on the amount of building blocks used per reaction and therefore the number of reaction steps, during which a replacement building block is introduced. Typical: 102 up to 105 compounds.

Keywords: Computational chemistry; Drug discovery

Introduction

Basic idea of combinatorial chemistry

Preparation of an outsized number of various compounds at an equivalent time.

High throughput- screening provides the foremost promising substances Combinatorial Chemistry as a valuable tool in drug discovery and material science Combinatorial Chemistry features a valuable tool in drug discovery and material science.

Distinction: Scaffold- based vs. Backbone- based libraries

Scaffold- based libraries

Definition: Core- structure, which all compounds of the library have in common. Scaffold can contain several single building blocks (here: amino acid and aminobenzophenone).

Backbone- based libraries

Lead identification & lead optimization e.g. within the drug discovery process. The development of latest processes for the generation of collection of structurally related compounds (libraries) with the introduction of combinatorial approaches has revitalized random screening as a paradigm for drug discovery and has raised enormous excitement about the likelihood of finding new and valuable drugs briefly times and at reasonable costs.

Advantages

(1) The creation of huge libraries of molecules during a short time is that the main advantage of combinatorial chemistry over traditional.

(2) Compounds that can't be synthesized using traditional methods of medicinal chemistry are often synthesized using combinatorial techniques.

(3) The cost of combinatorial chemistry library generation and analysis of said library is extremely high, but when considered on a per compound basis the worth is significantly lower in comparison to the value of individual synthesis.

(4) More opportunities to get lead compounds.

(5) Combinatorial chemistry accelerates drug discovery.

Disadvantages

(1) Though combinatorial chemistry would solve all the issues related to drug discovery, one still must synthesize the proper compound.

(2) There's a limit to the chemistry you'll do when using solid phase synthesis. The resin you employ is usually suffering from the reaction types available and care must be taken in order that the attachment of the reagent to the substrate and bead are unaffected. Each reaction step has got to be carefully

planned, and sometimes a reaction isn't available because the chemistry affects the resin.

(3) While an outsized number of compounds are created, the libraries created are often not focused enough to get a sufficient number of hits (library components whose activity exceeds a predefined, statistically relevant threshold) during an assay for biological activity. There's an excellent deal of diversity created, but rarely a central synthetic idea within the libraries. One can argue that there should be attention on the sort of molecule developed so as to maximise hits.

Conclusion

The Combinatorial Chemistry may be a methodology during which a really sizable amount of chemical entities are synthesized by condensing a little number of chemical compounds together altogether combinations defined by a little set of chemical reactions.

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