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Prespective

The DENDRAL: A Portmanteau of "Dendritic Algorithm" the Complete and Non-Redundant Generation of Molecular Formula

Rebecca Gonigle*

Department of Biological Sciences, University of Utah, Utah, United States

DESCRIPTION

According to a first-order analysis, all carbon-containing compounds that adhere to the Lewis electron pairing laws are included in the organic structure space. Practically, this is limited to excluding molecules with specific structural characteristics, such as those that make compounds unstable in water. The output molecules must be "meaningful" in terms of pharmacological space, for example, while considering this space. Most considerations of this space also involve some practical limitations. The size of the organic structure space is expected to be enormous. Organic structure space is complex, but organic formula space conceals this complexity by allowing a single molecular formula to represent a variety of structural isomers, even if the number of isomers per unique formula might vary greatly.

The abundance of chemical structures available today gives researchers in medicinal chemistry, pharmaceutical science, and biotechnology a virtually limitless number of options for creating novel medications and materials. A better understanding of life's biomolecular foundations in relation to the surrounding chemical space may be one key to understanding its origin. Life itself has probably optimised its biochemical processes throughout all stages of its evolution within the vast organic structure space available to it. The creation of algorithms for the enumeration of chemical space has always been strongly linked to NASA's exobiology efforts. The DENDRAL programme, a portmanteau of "dendritic algorithm," included the complete and non-redundant generation of all connectivity isomers corresponding to a given molecular formula. Mathematicians contributed new techniques to boost the effectiveness of the initial approaches, and starting in the 1990s, implementations became accessible as software packages for personal computers. Although the range of their possible use is far larger, these approaches have recently been rediscovered for use in astrobiology and origins of life research, specifically for the generation and analysis of virtual chemical compound libraries of amino acids and nucleotide analogues. In many different environments throughout the Universe, abiotic organic synthesis takes place. While the organic catalogues for some of these environments, like the interstellar medium, are rather limited (on the order of 190 distinct structures from mass 13 to 840 amu (see, for example), others are very complex. For instance, new research on carbonaceous chondrites suggests that there may be between 14,000 and 50,000 distinct organic compounds with unique molecular formulas (across the mass range of 150 to 1000 amu), which might be equivalent to several million distinct chemical structures.

Research evaluating the results of Miller-Urey electric discharge experiments using analogous methods], Hydrogen Cyanide (HCN) polymers and titan tholins have both discovered a significant number of novel formulas. Since there is a great deal of structural isomerism in organic chemistry, even though one-dimensional high-resolution mass spectrometry is able to determine exact masses and thus molecular formulae with a high degree of accuracy, each detected unique formula may instead be representative of an as-yet-unknown number of structural isomers. It should be mentioned that a further effective method that may be utilised to identify structural isomers is the mass fragmentation spectrum.

Correspondence to: Rebecca Gonigle, Department of Biological Sciences, University of Utah, Utah, United States, Email: rebecca.g@email.com

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