

有机化合物分子式的组合方式和分布规律的研究及其应用

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摘要 多年的观察和研究初步证实,自然界有机化合物可能存在的合理分子式在种类和数量上是有限和可知的,对分子量1000以下的分子式范围提出了符合实际的界定方法和计算式。据此已经人工书写或计算机打印出分子量16~800、只含C、H、O、N的分子式203470个,初步估算分子量到1000时共有分子式474000个。若以分子量为横坐标,分子式中的碳原子数为纵坐标作图,除个别外,这些分子式均分布在坐标系的一个三角形区域内,因而称其为三角形分布。但这只是自然界有机化合物分子式的一部分,全部则可能为流线形分布,三角形为流线形的头部。有机化合物分子式的三角形分布为有机化学家提供了有机分子式的预测、仪器测试结果的评判以及积极参与分子式的决定的主动能力,一改从前只能接受仪器测试结果的被动局面,从而加快了分子结构测定的速度。有机化合物分子式范围的界定和分子式的预测也为今后分子结构的界定和预测打下了初步基础。

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Abstract Study and Application on the Compositive Pattern and the Distribution of Molecular Formulas of Organic Compounds\$\$\$\$Cong Puzhu(Institute of Medicinal Plant Development,Chinese Academy of Medical Sciences, Beijing 100094,China)Abstract:Limitation and knowability on possible and rational molecular formulas of natural organic compounds are preliminarily discovered in kinds and quantities based on our researches for years. The delimitate schemes and calculating formulas corresponding to objective realities for the range of molecular formulas below 1000 of molecular weight are tentatively proposed. 203470 molecular formulas which contain only C,H,O,N four elements and molecular weight is from 16 to 800 have been written manually or printed by computer and about 474000 molecular formulas for molecular weight up to 1000 are evaluated. A triangle area which the most of molecular formulas is distributed in it comes out in a coordinate system if the abscissa stands for molecular weight and the ordinate for carbon atomic number in molecular formulas. The triangle,as a head,however,will be a part of whole molecular formula distribution, perhaps as a streamline. Organic chemists will have the initiative in evaluation of experiment data from instruments,calculation of molecular formula according to the delimitate formulas and final determination of them,change the former passive position just accepting experiment data and raise the efficiency of organic molecular structure elucidation if the technique is adopted. The primary foundation for future delimitate and calculation of organic molecular structure will also be laid on the range delimitate and calculation of molecular formulas. Keywords: molecular formula calculation, triangle distribution,application

Key words

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