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Molecular Diversity Preservation Strategies: The Proposal

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Abstract: Chemical samples constitute the precious molecular diversity. The basic idea of the molecular diversity preservation project MDPI launched in 1995 to preserve and explore it was introduced.

Keywords: Molecular diversity, chemical samples, chemical information.

Introduction

Recently, molecular diversity has been a topic of great interest [1, 2]. Techniques of combinatorial chemical libraries [2] have been developed to provide millions of compounds for pharmaceutical studies. Among many of their advantages, the similarity and the gradual variation of structures of the chemical species in combinatorial chemical libraries permit adjustments designed to optimize structure-activity relationships. However, as I have recently argued [3, 4], the high quality of a chemical species library relies on the distinct differences of both the structures and properties of the collected compounds. These compounds in isolated form are traditionally and still routinely prepared in the laboratories and isolated from natural sources.

The Proposal

The motive of this proposal stems from the observation of our practice as chemists that even though a large number of chemical species are generated around the world everyday, virtually all of them are almost simultaneously lost. Traditionally a chemical synthesis is carried out for a target compound. Consequently no precursors prepared as intermediates are regarded as worthy to be preserved. Sometimes a compound is prepared for very specific academic and industrial purposes such as a spectroscopic measurement or an enzyme-ligand binding test. Afterwards the samples may be regarded as useless and have to be discarded. In many cases such as the termination of a research project, graduation of a student, and retirement of a chemist or a professor, all the pertinent compounds accumulated may have to be discarded. This is a tremendous waste of both intellectual and human resources and a pitiful loss of the precious, high-quality molecular diversity [4].

The objective of this proposal is towards the substantial preservation of chemical species synthesized in chemical laboratories and separated and isolated from natural sources such as plants and animals. I would like to appeal to colleagues and endeavor to start the co-ordination of the following activities:

1. Organize a non-profit and independent body with the easy and free participation of all the personnel in both academic and industrial, and international chemical communities. The Organization can be called Molecular Diversity Preservation International [5].

2. Set up a permanent chemical species collection center or centers for world-wide, systematic collection of all the well-characterized, pure chemical species, including all the intermediates, donated by anybody in the world. They should not be commercially easily available compounds. The amount of a sample can be in the

range of 100g to 0.1g (or even less). To ensure that there are always the listed samples available, only a certain amount (e.g., no more than 90%) of a collected compound can be removed from the center for use. A nominal cost for use of these compounds will be charged to cover the expenditure of the Organization and to reward the original donors [5].

3. Publish *Molecules* [5]. The papers submitted for publication are accepted for publication only if the chemical species described there are correctly donated and deposited in a preservation center [6]. Because it may happen that a chemist obtained an interesting compound but the preparation can never be repeated or the yield is very low, such specimens are also to be collected if the supporting physical data are satisfactory. If the synthetic work is already published in a scientific journal, only the physical data will be presented, and a brief, schematic description of the synthetic route and purification procedure might be preferable. Otherwise a report may be prepared in a similar style as organic synthesis articles if the work has not been published before. This publication can be distributed at a reasonable price. [7].

The advantage of our strategy is that the contributors take a certain responsibility for the quality of the compounds which will have been adequately described in the articles in *Molecules*. This publication can also serve as an advertisement to promote exchange and application of the available compounds [7].

4. Set up a database for the compound collection [5].

5. Management will be carried out with the connection and possible supervision of an international organization such as the World Intellectual Property Organization of the United Nations in Geneva, to achieve as fair and broad as possible use of this intellectual treasure. The experiences of biodiversity preservation such as seed and micro-organism collections in many countries, might be in this context useful [8, 9].

Concluding Remarks

I hope this effort will prevent further loss of molecular diversity created in our laboratories. In addition, this will enable the laborious and intellectual contributions of chemists to be fully appreciated and benefited by the whole humankind. Despite many potential difficulties, I think this proposal will work if this can be supported by my colleagues.

Great progresses have been made so far for the *Molecules*/MDPI project [5].

References and Notes

[1] This proposal was sent to many chemists worldwide on 27 March 1995. For a original version of this proposal, please visit: http://www.mdpi.org/proposal.htm.

[2] Felder, E. R. The challenge of preparing and testing combinatorial compound libraries in the fast lane, at the front end of drug development. *Chimia*, **1994**, *48*, 531-541.

[3] Lin, S. -K. Correlation of entropy with similarity and symmetry, *J. Chem. Inf. Comp. Sci.* **1996**, *36*, 367-376.

[4] Lin, S. -K. Molecular diversity assessment: Logarithmic relations of information and species diversity and logarithmic relations of entropy and indistinguishability after rejection of Gibbs paradox of entropy of mixing. *Molecules* **1996**, *1*, 57-67. (The electronic version of reprint of this published paper can be downloaded from http://www.mdpi.org/lin.htm)..

[5] Lin, S. -K. *Molecular Diversity Preservation Strategies: Actions*, presented at The First Electronic Molecular Modelling & Graphics Society Conference will be held in October 1996. For the recent progresses, see: Lin, S. -K. On the Chemical Samples Exchange, paper presented at ECSOC-1, September 1-30, 1997.

[6] This very strict condition is changed to the following: *Molecules* encourages authors to deposit their compound samples at MDPI center in Switzerland and distribute at reasonable prices worldwide. Contributions of papers only and compounds only are also welcomed (also ref. 5).

[7] For up-to-date information regarding this new journal, please visit http://www.mdpi.org/molecules.

[8] World Intellectual Property Organization, *Guide to the Deposit of Microorganisms under the Budapest Treaty*, WIPO Publication No. 661 (E), Geneva: WIPO, Reprinted 1994.

[9] (a) Lin, S. -K. *Guide to the Deposit of and Exchange of Compound Samples*, ACS 212th National Meeting, Orlando, Florida, August 25-29, 1996. (b) Lin, S. -K. Molecular Diversity Preservation Strategies: The MDPI Project, presented the 36th IUPAC Congress - organized by the New Swiss Chemical Society. Geneva, Switzerland. August 17 - 22, 1997. The abstract was published: Lin, S. -K. Molecular Diversity Preservation Strategies: The MDPI Project, *Chimia*, **1997**, *51*, 544.

Comments

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