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On the Chemical Samples Exchange

Shu-Kun Lin

Molecular Diversity Preservation International ([MDPI](http://www.mdpi.org/)), Saengergasse 25, CH-4054 Basel, Switzerland; Phone +41 79 322 3379; Fax +41 61 302 8918; E-mail: Lin@mdpi.org, <http://mdpi.org/lin.htm>

With [biographical summary](#)

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Abstract: Chemical information and chemical samples constitute the precious molecular diversity. The molecular diversity preservation project MDPI was launched in 1995 to preserve and explore them by worldwide samples exchange.

Keywords: Molecular diversity, chemical samples, samples exchange

Introduction

The acquisition of chemical samples by collection and combinatorial synthesis has now become the bottleneck in the process of new drug discovery. As a chemist who worked on several drug discovery projects [1] and during those years as an organic chemistry student, I frequently observed that the final work of a retiring chemistry professor in a university or a retiring chemist in a company was trashing their collected compounds. Even chemists who have just completed a research project, and need storage space for newcomers or new projects, throw away old compounds. If they synthesize a target product, they normally do not keep any by-products or any small amounts of intermediates.

A proposal was prepared after many discussions with my colleagues, particularly chemists in Basel. The proposal [2] distributed to many chemists in March 1995 received numerous very encouraging and positive responses. Therefore, I started to realize the ideas step by step. With strong support from chemists from both the academic and the industrial side, and help from local government and the World Intellectual Property Organisation of the United Nations in Geneva, we have made great progresses so far, which is reported herewith.

Actions

First, we announced the MDPI activities in a chemistry journal [3].

Chemists contribute not only new knowledge but also new substances. We launched the first journal of organic chemistry and natural product chemistry, [Molecules](http://www.mdpi.org/molecules/) (visit <http://www.mdpi.org/molecules/>), that encourages authors to register or deposit their compound samples at MDPI center in Switzerland and distribute at reasonable prices worldwide. The idea of this program is to supply both chemical information as well as the chemical substances themselves. Contributions of papers only and compounds only are also welcomed. Following the example of *Molecules*, several other chemistry journals started to support MDPI efforts by adding at their *Information for Authors* the following message: "**Samples Exchange:** Authors may register or deposit their available compound samples at MDPI in Switzerland. For more information, visit <http://www.mdpi.org/> or contact MDPI Center, Saengergasse 25, CH-4054 Basel, Switzerland. tel. +41 79 322 3379, fax +41 61 302 8918, email: info@mdpi.org."

Acta Chimica Scandinavica

Anales de Quimica International Edition (Springer)

Catalysis Today (Elsevier)

Chemia (No.3/1997 page 112, published by New Swiss Chemical Society) Editor-in-Chief, Prof. Dr. Camille Ganter, Lab. f. org. Chemie, ETH-Zuerich, CH-8092 Zuerich, Tel. +41 1 632 2900, fax. +41 1 632 1072, e-mail: ganter@org.chem.ethz.ch

Journal of Macromolecular Sciences-Review in Macromolecular Chemistry and Physics (Marcel Dekker, Inc.)

Journal of Peptide Science (Wiley)

Organic Preparations and Procedures International (OPPI Inc.)

Even though there are several urgent legal issues in this unprecedented project which need to be carefully considered, we suggest that those MDPI-registered samples requested and used should be treated by the users as if the samples were obtained according to published literature, specifically *Molecules* or therein relevant cited reference(s), including patents [4,5].

MDPI coordinates world-wide collection, storage and exchange of synthetic and natural compounds. We ask retiring professors or chemists who have just completed a research project not to throw away their compounds. When they synthesize a target product, they should keep any by-products and small amounts of intermediates. The amounts of the compound samples (100 mg-100 g each, smaller amounts also acceptable) are flexible. Alternatively, if they have a large number of compounds, MDPI may register them into [MDPI available compounds databases](http://mdpi.org/mdpi/database.htm) (visit <http://mdpi.org/mdpi/database.htm>) and provide distribution services. The contributors' names are released in the database, because they are responsible for the quality of the samples. The unit prices for sample services are also published in the database so that the amount of the reward to the sample contributors can be easily and fairly estimated.

The MDPI storage center in Switzerland has also been set up and is supervised by a chemist.

We also have actively contacted with World Intellectual Property Organization of the United Nations in Geneva, and found that the experiences of biodiversity preservation such as seed and micro-organism collections in many countries, might be useful in this context [6]. Thus, learning from biodiversity preservation experiences, these actions have been taken to preserve molecular diversity worldwide.

Discussion

Sample Stability

The stability of samples and the purity of old compound samples have been the main concern of many chemists. We found that in many pharmaceutical companies, all the solid samples prepared more than 50 years ago and stored even at room temperature have so far been found to be applicable and can be used for such purposes as high throughput screening. Many of the MDPI compounds can be used for high throughput screening where several compounds are mixed by the users before the bioactivity tests. The possible impurities in a sample are not a problem for such tests. According to our investigations, many chemical reagent suppliers store most of their chemicals at rt for several years. The decay of compounds is greatly accelerated only if they are exposed to air, light, or are not in solid form.

Legal Problems

This problem was also discussed in the "Chemistry and Law Section" of the ACS 212th National Meeting [4b] and in IUPAC congress [5].

References and Notes

1. E.g., S. -K. Lin, V. Rasetti, Synthesis of Benzospiro[5,6]undecane Derivatives as Inhibitors of Steroid 5- α -Reductase, *Helvetica Chimica Acta*, **1995**, *78*, 857-865).
2. Lin, S. -K. [Molecular Diversity Preservation Strategies: The Proposal](#), paper presented at ECSOC-1,

September 1-30, 1997. This was first presented at The First Electronic Molecular Modelling & Graphics Society Conference, held in October 1996.

3. The [MDPI Announcement](#) was first published in *Synthesis*, **1995**, No.9, 10 and 11, **1996**, No.4 and 5.
 4. (a) Lin, S. -K. [Guide to the Deposit of and Exchange of Compound Samples](#), presented twice at the Chemical Information Section of the ACS 212th National Meeting, Orlando, Florida, August 25-29, 1996. (b) This paper was also presented orally at the "Chemistry and Law Section" of the ACS 212th National Meeting.
 5. (a) 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. (b) Lin, S. -K. Molecular Diversity Preservation Strategies: The MDPI Project, *Chimia*, **1997**, 51, 544.
 6. World Intellectual Property Organization, *Guide to the Deposit of Microorganisms under the Budapest Treaty*, WIPO Publication No. 661 (E), Geneva: WIPO, Reprinted 1994.
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[Shu-Kun Lin](#)

Shu-Kun born March 24, 1957 in Hanchuan, Hubei Province, China. He graduated from Wuhan University in 1982, majoring inorganic chemistry. He studied physical chemistry in the Chinese Academy of Sciences (1982-1986, MSc in 1985) and in the USA (1.1987-7.1989). He obtained his doctorate in organic chemistry at the Swiss Federal Institute of Technology (ETH-Zurich) in 1992 after three years studies at the group of Prof. Dr. Bernhard Jaun, Lab. f. org. Chemie-ETH-Zurich. He then worked at Ciba-Geigy Ltd. for ca. three years, first as a postdoctoral research associate in organic synthesis and worked on two drug discovery programmes in the CNS area for 1.5 years, secondly for the Dyestuffs Division of Ciba-Geigy Ltd., receiving training in dyestuff R&D and Production. He initiated a molecular diversity preservation project and founded [MDPI \(Molecular Diversity Preservation International\)](#), a nonprofit and independent international organization in Switzerland. In 1995 he launched the first journal [Molecules](#) that encourages authors to deposit their compound samples. He is the main author of 40 publications. He has two children (a daughter Qian-Qian, born July 27, 1986, and a son, Di-Fan, born June 1, 1996). His personal website is <http://www.mdpi.org/lin.htm>. Present Address: Dr. Shu-Kun Lin, Molecular Diversity Preservation International (MDPI), Saengergasse 25, CH-4054 Basel, Switzerland. Tel. +41 79 322 3379, Fax +41 61 302 8918, E-mail: Lin@mdpi.org.

Comments

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