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MolBank: Rapid and Easy Publication of Short Notes of Individual Molecules

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Abstract: Experimental data of organic synthesis and compound analysis is very precious chemical information. The monthly chemistry journal *Molecules*' new column "MolBank" was launched in April 1997 to preserve a large amount of experimental data of organic synthesis and structural characterization works of individual molecules, which have been conventionally unpublishable.

Keywords: Molecular diversity, chemical information, MolBank.

Introduction

Now, small pieces of experimental work of individual compound preparation and structural characterization can be rapidly and easily published in the MolBank column of the monthly chemistry journal [Molecules](http://www.mdpi.org/) [1,2]. Five issues of this column have been published up to August 1997. So far many small pieces of experimental findings have not been recorded in the literature. This is a tremendous loss of useful chemical information. We believe the publication of the MolBank column in *Molecules* is a very significant step towards the preservation of molecular diversity of precious experimental findings.

The Loss of Chemical Information

Unlike other fields of science, chemists contribute a large volume of knowledge (chemical information) based on *experimental* data [3].

Many chemists working in industry research and development have accumulated a large amount of synthetic and structural characterization results. However, many of them have never been published. It is understandable that if the chemists have done a good job and are well-paid, both sides, the chemists themselves and the companies are satisfied. They do not need to publish anything. Their interests in publishing their works are further discouraged by the conventional standard of chemical paper publications: they do not want to spend a lot of time painstakingly preparing the "introduction" and the "discussion" sections required by conventional chemistry journals. The preparation of these two sections are tricky. Many very good experimental works have been rejected because the authors failed to prepare good paragraphs for these sections. Even published "experimental work" can be published virtually without any experimental data presented if you are a good writer: It is not rare in some prestigious journals of chemistry to find papers without any experimental data except a statement such as "all the compounds give satisfactory elemental analysis (C,N,H), IR and NMR" [4-6].

For similar reasons, chemists in universities also have this problem and feel reluctant to publish fully their experimental findings, particularly if they are scattered unassembled experimental data of individual compounds.

Therefore, most (I estimate at least 2/3) of the experimental data for organic molecules was previously never published.

On the other hand, we know that chemistry is a typical experimental science. Chemical knowledge as written in the text books is based on experimental findings. The recording as fully as possible of all these experimental findings would on any account be very useful.

Can we do something about this?

Molbank

Starting with volume 2 of the journal *Molecules* [1], the nonprofit international organization MDPI will provide, in addition to the sample deposit services, the service for the deposit of information (experimental data, particularly synthesis and spectroscopic data). Preserving and exploiting molecular diversity for both information and samples will continue to be the goal of the journal *Molecules* and the organization MDPI.

Authors are not required to prepare "introduction" and "discussion" parts - it is not necessary to be asked to tell why you want to prepare these compounds.

Molbank papers are short notes of synthetic works and the data of the structural characterization which can be one molecule (one structure) per paper and can be as short as one page only. Such publications in *Molecules* will serve as the experimental data deposit.

This project is interesting because a large volume of very precious chemical information, particularly the very diverse works of synthesis and structural characterization have either never been published -- the submitted papers were rejected by editors because they were too trivial (normally because it belonged to the classical scope of chemistry, i.e., pure synthetic or pure spectroscopic measurements), or the chemists themselves never planned to publish such works for individual compounds and isolated data because they thought them not publishable in a traditional journal. We believe that synthesis and structural elucidation of individual compounds are still the essence of chemistry and the material foundation of other research.

The ready publication of all scattered unassembled data for individual compounds in *Molecules* as short posters will provide a bank for chemists to deposit all of their information of synthesis and structural characterization, together with the sample availability information. Those works that have no compound samples available will also be published. When a large volume of (say 1 million) structures is published in this way and also constructed as a retrievable databank, it will be a very useful treasure to all chemists and other related scientists. If every synthetic chemist contributes 100 such posters, this number will be easily reached within several years.

Discussion

Many colleagues may think that it is not interesting and worthwhile to publish solely a large volume of experimental findings. However, there are several strong reasons. Firstly, the priority of the synthetic work and characterization of the compounds will be recorded in the literature as the work performed by the author. Secondly, these publications will be greatly appreciated by other experimentalists: the experimental results published will be very useful for others to prepare the samples and the similar compounds [6]. Finally, it should be our obligation and duty to preserve as complete as possible all the experimental findings.

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References and Notes

1. Molbank website: <http://www.mdpi.org/molbank/>.
2. See also an editorial: S. -K. Lin, Preserving and Exploiting Molecular Diversity: Deposit and Exchange of Chemical Information and Chemical Samples. *Molecules* **1997**, *2*, 1-2.

(<http://www.mdpi.org/molecules/edito197.htm>)

3. Lin, S. -K. Chemical information. *Chem. Eng. News* **May 26, 1997**, 4.

4. The "high yield" standard is another questionable standard for many publishable synthetic works [5]. As a reasonably skillful synthetic organic experimentalist, I found quite a number of papers that claimed (higher) yields which can never be reproduced. Normally 20% higher than what I find if I repeat a synthesis. Therefore, my chemistry journal *Molecules* does not set the "high yield" as a high standard of organic synthesis [5] and authors can be encouraged to be honest and to report reproducible yields.

5. See also an editorial: S. -K. Lin, A Good Yield and a High Standard. *Molecules* **1996**, 1, 1-2.
(<http://www.mdpi.org/molecules/edito96.htm>)

6. As a synthetic organic chemist, I may read carefully only the experimental section, sometimes making a Xerox copy of only the specific experimental paragraphs of a paper or a patent.

Comments

During 1-30 September 1997, all comments on this poster should be sent by e-mail to ecsoc@listserv.arizona.edu with **F0001** as the message subject of your e-mail. After the conference, please send all the comments and reprints requests to the author(s).
