

[E0006]

MolBank: First Fully Web-Based Publication of Chemical Reaction Data

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Abstract: We report the experience and the recent improvement of the [MolBank](http://www.molbank.org) section at the <http://www.molbank.org> server and the journal *Molecules* (<http://www.mdpi.org/molecules/>, ISSN 1420-3049). The monthly chemistry journal *Molecules*' new column "MolBank" was launched in 1997 to publish short notes of one-paper one-page for one structure.

Keywords: Chemical information, chemical journal, MolBank, online journal, structure search, substructure search, online submission.

Introduction

There are some very exciting new development regarding MolBank section of *Molecules*. Mainly we have the new <http://www.molbank.org> server [1,2] and have 2D substructure and structure search function and web-based paper submission capacity, in addition to many other new features. We presented this results at the 218th ACS National Meeting August 22-26, 1999 (Figure 1) [3].



Figure 1. Shu-Kun Lin and Luc Patiny at the 218th ACS National Meeting August 22-26, 1999. We presented this paper there also.

We report the experience and the recent improvement of the MolBank section and the journal *Molecules* here.

MolBank Section [4]

Molecules (<http://www.mdpi.org/molecules/>, ISSN 1420-3049) publishes in the section of [MolBank](http://www.molbank.org)

(<http://www.mdpi.org/molbank>) very short notes of experimental data records for individual molecules. Any scattered, unassembled experimental data for individual compounds which is conventionally not publishable is particularly welcomed, to be published as one-paper one-page for one structure and given special page numbers (M1, M2, etc.). They have been published in HTML format, with at least a formula of the target molecule. MDL MOL file is also included for every MolBank short notes. All papers submitted for consideration and publication in this column of "MolBank" have been refereed and the accepted papers edited (English corrected and format unified). The related chemical samples are in most cases available and the availability information is also published. All papers published in the MolBank section have been indexed and abstracted by several leading indexing and abstracting services, including Chemical Abstracts; CAPLUS; Science Citation Index Expanded; SciSearch, Research Alert; Chemistry Citation Index; Current Contents/Physical, Chemical & Earth Sciences. *Molecules* is the first online publication of experimental chemistry [5-7].

New Development

The MolBank section (<http://www.molbank.org>) of *Molecules* is perhaps the first, almost perfect electronic journal in chemistry. You can already search on the website www.molbank.org all the published compounds by 2D substructure search.

MolBank new features:

- easy, electronic procedure to submit a paper
- free access from the Internet with powerful searching tools
- IUPAC Names (for the titles) generated by CAD (<http://www.acdlabs.com>) in addition to the following
- one-paper for one reaction with one fully characterized product
- very fast publication, particularly suitable for publishing short communications to have the priority the a chemist is the first to have synthesized a compound or have fully characterized a natural product
- easy publication of short notes of scattered unassembled experimental data for individual compounds which is conventionally not publishable.

Dr. Luc Patiny started to serve as the MolBank section Editor of MOLECULES (<http://www.mdpi.org/molecules/editors.htm#molbank>) in August 1999. Dr. Patiny is from the Institute of Organic Chemistry, University Lausanne, Switzerland.

For more information, visit the <http://www.molbank.org/> website.

References and Notes

1. MolBank official website is <http://www.mdpi.org/molbank/>.
2. MolBank server <http://www.molbank.org/> has the MolBank section papers in searchable database form. The web-based submission and reviewing systems are also installed there.
3. Lin, S.-K.; Patiny, L. *MolBank: Preservation and Publication of Chemical Reaction Data*. Paper presented at the 218th ACS National Meeting August 22-26, 1999.
4. Lin, S.-K. *MolBank: Rapid and Easy Publication of Short Notes of Individual Molecules*. Paper presented at the First International Electronic Conference on Synthetic Organic Chemistry (ECSOC-1), www.mdpi.org/ecsoc/, September 1-30, 1997.
5. 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>)
6. Lin, S. -K. Chemical information. *Chem. Eng. News* **May 26, 1997**, 4.
7. 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>)

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