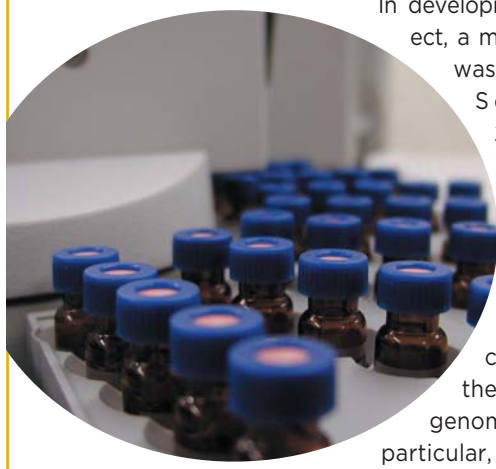
Post Genomic Chemistry

More than 20 specialists from 11 countries (Belgium, Canada, Estonia, France, Germany, Italy, Poland, Russia, Sweden, UK, and USA) actively participated in an interdisciplinary project on post genomic chemistry. In developing this project, scientists joined forces from the fields of structural chemistry, biopolymer science, synthetic chemistry, drug design, and bio-inorganic and bio-analytical chemistry.

These scientists prepared a technical project report, which has been submitted to *Pure and Applied Chemistry* for publication, based on their published research from the last two to three years in journals such as *Nature*, *Science*, *Journal of American Chemical Society*, *Journal of Analytical Chemistry*, *Journal of Molecular Catalysis*, and others.



In developing this project, a mini-workshop was held 6–8 September 2003 in Moscow, which allowed experts to exchange views on chemistry in the post genomic era. In particular, they discussed the implication of advances in genomics, proteomics, biomimetics, and biological and chemical informatics. Such advances involve combinatorial chemistry and automated chemical synthesis, synthesis of new classes of unnatural amino acids, development of new biosynthesis methods for preparation of proteins containing unnatural amino acids, chemical management of biosystems at the molecular level, and self-multiplying polymers.

In deciding on the project objectives, this group of scientists was influenced by a number of different conferences and seminars. Great interest was generated in particular by a plenary lecture on "Post Genomic Chemistry: New Possibilities and New Challenges" presented at the 17th International Mendeleev Congress on Pure and Applied Chemistry (September 2003, Kazan).

The development of this project revealed the necessity of creating new educational programs and training courses for chemistry students and faculty on the chemical basis of genomics. Such courses could include the chemical basis for genomic studies, genes and genomes for chemists, and bio- and chemo-informatics.

Financial support for the project was provided by IUPAC and the "Biocatalysis and Biocatalytical Technologies" project of the Ministry of Science and Technology of the Russian Federation.

For more information, contact the Task Group Chairman Sergey D. Varfolomeyev <sdvarf@enzyme.chem.msu.ru>.

www.iupac.org/projects/2001/2001-005-1-300.html

Analog-Based Drug Discovery

The Chemistry and Human Health Division Committee has reviewed the project proposal Analog-Based Drug Discovery and has approved the project as one of the divisional activities. The international teamwork started in January 2003. The project is part of the work of the Subcommittee on Medicinal Chemistry and Drug Development.

Analogs of drugs play an important role in the evolution of drug discoveries. Statistically, every second drug is an analog, therefore, it is of interest to analyze the relationship of these drugs to the pioneer discoveries and to each other.

The goal of this project is publication of a reference book for medicinal chemists and students that provides an easily usable overview of drug-analogs and their role in medicinal chemistry.

The book will consist of the following chapters, to be written by the persons listed:

- Introduction (Robin Ganellin)
- Optimizing Drug Therapy by Analogs (Janos Fischer)
- Analogs as Means of Discovering New Drugs (Camille G. Wermuth)
- Drug Likeness and Analog-Based Drug Discovery (John Proudfoot)
- Case Studies
  - —Lacidipine (Giovanni Gaviraghi)
  - —Pantoprazole (Jorg Senn-Bilfinger)
  - —Esomeprazole (Per Lindberg)
  - —Moxifloxacin (Uwe Petersen)
  - —Azithromycin (Miljenko Dumic)
  - —Drospirenone (Rudolf Wiechert)
  - —Bisphosphonates (Eli Breuer)
  - —Glucocorticoids (Zoltan Tuba)
- Table of Drug-Analogs (Janos Fischer)
- Subject Index

According to the schedule, the final manuscript will be ready by 30 June 2004. Proposals and further case studies are welcome.

For more information, contact the Task Group Chairman Janos Fischer <j.fischer@richter.hu>.

www.iupac.org/projects/2002/2002-051-1-700.html

Glossary for Chemists of Terms Used in Toxicology—Revision and Updating

Toxicology is a subject area dependent on good chemistry and that influences chemistry through its impact on legislation for chemical safety. For the development of both, it is essential that toxicologists should be able to communicate with chemists and that there should be a clear, common understanding of the meanings of key terms. This was recognized in 1993 when IUPAC published a "Glossary for Chemists of Terms Used in Toxicology" as an official recommendation in *Pure and Applied Chemistry*, and prepared for publication by J. H. Duffus.

The glossary was widely recognized as authoritative. In fact, it was adopted by the U. S. National Institutes of Health as the glossary for its TOXNET Web site. Since this Web site is now being updated, J. H. Duffus was asked if the existing glossary could be revised and brought up to date so that it could be incorporated into a new educational part of the site. Revision is necessary since toxicology has developed considerably in the 11 years since the glossary was first published. Already the need for a current glossary in toxicokinetics has been recognized by IUPAC in another project (project number #2000-034-2-700), which also be involved in the revision. It is proposed, as before, to seek input widely from international authorities, including the International Union of Toxicology. It is envisaged that the glossary in its revised version will cover all key terms relevant to toxicology in one source document making for ease of use. The terminology of risk assessment will also be included since application of toxicology in risk assessment is one of its most important uses.

For more information, contact the Task Group Chairman John H. Duffus <j.h.duffus@blueyonder.co.uk>.

www.iupac.org/projects/2003/2003-028-1-700.html

Structure and Properties of Polymer/Clay Nano-Composite Materials

Recent developments in the technology of inserting (intercalating) polymer chains in nano-scale layers of clay have produced new types of high-performance polymer composites. However, the effects of the higher order structure on mechanical properties are not yet well understood. For example, little is known about the crystallization of polymer chains confined in the nano-scale layers and subsequently occurring morphology formation. Since mechanical properties of the composites are strongly affected by the higher order structure, the control of the higher order structure becomes a key technology to design nano-composites with excellent performance and/or functions.

Barrier properties of the composite to various gas molecules are greatly improved by the exfoliated structure that occurs when the clay layers are completely separated by the polymer chain and the clay sheets in the nano-scale are dispersed throughout the polymer matrix. Only a small amount of clay is needed to reduce drastically the permeability of the nano-composite to oxygen and carbon dioxide. The composite could be used in food packaging applications, such as beer containers.

The purpose of this study is to clarify the relation-