

# IUPAC Division VII. Chemistry and Human Health

**Bureau Report: January – September, 2004**

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## **I. Executive Summary**

The merger of the former Medicinal Chemistry and Clinical Chemistry/Toxicology Sections into the Division of Chemistry and Human Health (VII) has proven to be an effective way for the IUPAC to oversee and allocate funding to all of these areas while using a condensed administrative infrastructure. To promote the core of expertise required to support the technical diversity afforded by these areas, Division VII, in turn, maintains three, standing Subcommittees led by appointed Chairpersons who are recognized internationally within each of their fields. These Subcommittees are Clinical Chemistry, Medicinal Chemistry, and Toxicology. An ad hoc Subcommittee, also led by an appointed Chairperson, has additionally been organized to deal with the IUPAC nomination and election processes for the Division. While a few members of each Subcommittee also sit on the Division Committee, the majority of the technical Subcommittee members are drawn as volunteers from each of these fields, respectively. The Election Committee has representation from all three areas.

The Subcommittees hold independent meetings on a regular basis and each Chairperson provides an update about their activities by either personally attending or forwarding a written report to the Division meetings which are held about twice a year. This focus of expertise coupled with the broader perspectives afforded during the Division meetings, has proven to be an effective way to encourage and initiate the evaluation of new IUPAC Project submissions, as well as to provide for assessments of ongoing projects and their subsequent impact. Final approval of new projects and additional tracking of ongoing projects, occur at the Divisional level wherein an equitable balance across all activities and the Division VII's IUPAC-allocated funds is sought among all three Subcommittees. Presently, Division VII is carrying 24 projects for which 2 are interdivisional, contributes to 2 additional interdivisional projects, and has 3 projects undergoing review for which 2 are interdivisional.

## **II. Activities Organized by the Six Goals of the IUPAC Strategic Plan**

*1. Provide leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences.*

Division VII's organization into three subcommittees allows this, as well as all of the other, strategic objectives to be focused within the contexts of Clinical Chemistry, Medicinal Chemistry and Toxicological Chemistry. Each subcommittee brings together a group of experts from around the globe to discuss items relevant to their area. For example, through such discussions, the Medicinal Chemistry group has determined that the global harmonization of patent laws impacting upon the pharmaceutical industry would benefit from a broad consideration of several issues. Toward that end, a project

proposal is presently being drafted to objectively address these issues by starting with a general survey that will be administered globally to a variety of scientists, practitioners and administrators for whom patents are an important aspect of their work.

*2. Facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.*

All three of Division VII's Subcommittees remain extremely active in producing glossaries and recommendations for standardization of terms within their respective areas. A quick scan down the list of completed, ongoing and proposed projects indicates our numerous activities in this area (see Section IV. Tabular Material).

Another type of tool that Division VII is constructing in conjunction with the IUPHAR and the latter's initial funding supplied by the ICSU, is an Internet database that will contain human drug metabolism data and will, in turn, be made available to users across the globe via a non-profit basis. With an emphasis on the chemical structures for both the parent drug or xenobiotic and the various metabolic biotransformation products, the Human Drug Metabolism Database (hDMdb) database will be extremely useful to both the medicinal and toxicological chemistry arenas. It is interesting to note that while Division VII has already been working on this project for four years, the importance of such projects within the chemical community is only just now beginning to be fully appreciated. For example, statements quoted in the recent *C&E News* (June 28, 2004 pages 37-41) article that highlighted an international conference dedicated to 'Charting Chemical Space: Finding New Tools To Explore Biology' indicate that one of the 'grand challenges' elaborated by Stuart Schreiber and several other well-recognized scientists was an outright appeal for the production of open databases having chemical structures connected to biological properties.

*3. Assist the chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life.*

Moving forward from one of its earlier publications ('Medicinal Chemistry in the Development of Societies: Biodiversity and Natural Products,' *Eur. J. Med. Chem.*, **32**, 2000, pages 1121-1125) which specifically addresses the critical role that the pharmaceutical industry can play in developing nations, Division VII is now undertaking follow-up projects that intend to bring workshops on this topic to such countries. Our initial program will target the pharmaceutical industry in India which has heretofore been able to establish strengths in process (scale-up) chemistry but not in the earlier stages of drug discovery and invention, despite their long history with natural product-based remedies and herbal medicines. This undertaking may also be applicable to China and many other Eastern countries. Even less developed nations are being targeted in a somewhat different manner (see Strategic Goal 4.)

*4. Foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.*

The aforementioned hDMdb project is also applicable to this goal. For example, during a poster presentation about this project at the recent International Society for the Study of Xenobiotics (ISSX) meeting (Vancouver, September, 2004), its 'free-access-for-all' principle was applauded by several scientists from less developed nations who happened to have become engaged in a broader discourse with scientists from some advanced countries who wanted to know if the database might be able to be commercialized so as to generate funding that could move its development along at a faster pace (but with the inherent principle then falling into place that the db would thus be made available only to those who could afford to purchase it).

Continuing from Strategic Goal 3, we have determined that the best follow-up to our earlier publications for countries which are in the very early stages of development in that they completely lack any type of sophisticated chemical industry infrastructure, needs to be approached at a more fundamental level, i.e. by educational programs directed through their budding academic institutions rather than at the industrial level. Division VII's ongoing projects on basic clinical/medicinal/toxicological chemistry education within the Latin America region represents an initiative along these lines.

I assume similar to all of the other Divisions, Division VII repeatedly votes in favor of IUPAC sponsorship of meetings and conferences applicable to our area whenever they are to be organized or hosted by less developed nations and wherein the caliber of the related chemical technologies is to be held in the highest regard. During the last year, Division VII has favorably reacted to about two of such requests each quarter.

*5. Utilize the IUPAC's global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.*

Ongoing chemical education initiatives pertinent to human health have been described above for audiences in industry (Strategic Goal 3) and academia (Strategic Goal 4). For the public at large, two additional initiatives deserve mention. First, as a follow-up to our prior, somewhat technical article ('Natural and Non-natural Substances Related to Human Health,' *PAC*, **74**, 2002, pages 1957-1985) Division VII produced a summary version which compares the attributes of synthesized drug versus natural sources for chemical compounds in laypersons terms. Subsequent to publication of the latter in *CI*, this has now been picked-up within the lay press with translations being effected by other countries as evidenced by the entries noted on the Web-based, Eureka Alert Service.

The second initiative to be mentioned in this regard is a project submission that is under review entitled 'Molecular Gastronomy.' The end-product from this project will be a short monograph wherein the point will be made clear that when a person undertakes everyday cooking, they are indeed practicing chemistry and that in the process of trying to improve palatability, various procedures can also either enhance or diminish the overall nutritional and/or medicinal value of a given food item or dietary supplement.

*6. Broaden national membership base and seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender and age.*

One of the new project criteria that Division VII has laid in place from the onset during the Subcommittee meetings and then further reinforces at the Divisional level, is that the proposed project participants list reflects the exact spirit conveyed by this final IUPAC strategic goal. That these participants might then become future members in various IUPAC bodies provides a grass-roots technical approach toward accomplishing this end. Exemplifying this scenario is the fact that the current President of Division VII first became involved with the IUPAC via an invitation to participate on a project about eight years ago and has gradually become more and more active. The same philosophy has been applied to the Subcommittee charged with the Division VII-related nomination and election processes, although in this case there is the possibility that a new member might become immediately involved at a higher administrative level within the IUPAC infrastructure.

In terms of seeking younger members (also applicable to Strategic Goal 5.), Division VII had the pleasant experience of hosting a 'Young Observer' during the Ottawa meeting. To further support this program, Division VII subsequently encouraged this individual to seek IUPAC sponsorship for a symposium that he was trying to set-up in his country. This has all occurred favorably and a full set of proceeding papers covering the symposium's cutting-edge chemistry in the area of nuclear delivery and functional modification by small molecules will soon be published in PAC. It is hoped that through such mentoring, this young and rising investigator will gradually become more and more active within the IUPAC as well.

### **III. Challenges, Problems and Solutions**

Within this topic, Division VII would like to suggest one item for potential discussion, namely 'additional financing mechanisms for the Divisions.' The problem that Division VII has is that its IUPAC budget gets spread very thin based just upon its technical projects load which, in turn, makes it difficult for the Division to optimize certain administrative activities or to embark upon new recruitment initiatives (the latter presumably being an ongoing challenge for everyone within IUPAC in terms of either getting new members or new projects or both). A brief summary (proposal or potential solution) follows.

We propose that in addition to the current, projects-based funding mechanism (with the presently recommended bump-up percentage allocated for administration), Divisions be allowed to also obtain additional funds via two new mechanisms: (1) Recouping a share of any royalties on published books, monographs etc. for which they were responsible for generating, e.g. a 75/25 split with the IUPAC first receiving all of such funds and then, after deducting any cost outlays that they may have incurred including that of the initial money the IUPAC allocated via the Division to the relevant project at its outset, distributing 75 % of such remaining monies to the appropriate Division; and, (2) Receiving a share of any monies obtained by their own efforts toward fund raising, e.g.

again a 75/25 split with the money initially to be received by the IUPAC but then immediately divided such that 75 % goes directly to the Division since the IUPAC will have had no overhead for any of such initiative that would need to be first accounted for.

These monies should be for unrestricted use by each Division with the only provisos being that the money must in some way be directed toward the IUPAC Strategic Goals and, obviously, can not be used for any person's or entity's profit. For example, in the case of Division VII, we would like to use such funds to be able to pay for the expenses for additional people to attend our Subcommittee and Divisional meetings, which, as alluded to in the Executive Summary, become the drivers for all of our efforts in general and, as clearly indicated in Section II, Goals 4, 5 and 6 represent a very specific, grass-roots approach toward engaging our relevant chemical communities and recruiting new participants. Such funding could be particularly valuable for the latter when further directed toward recruitment of scientists from less developed nations and of young (not yet well-established) scientists, both of whom are likely to have financial difficulties of their own.

One of the benefits of undertaking fund-raising at the Divisional level is that it can be pursued from one technical expert to another identical technical expert (IUPAC Division person to industry person) with the reasons for encouraging an interaction then being able to be built-up from a very common base. One of the challenges will be to coordinate such activities with the IUPAC National Adhering Organizations who may also be attempting to conduct such fund-raising. In the States, the NAO has such a program but it is administrator to administrator and it appears to be having little success. I plan to attend their next meeting (November) to see how we might either work together or move independently in this regard. However, since the same issue could arise in other countries as well, an over-riding policy/directive from the IUPAC itself becomes a more efficient and uniform way to address this aspect of the proposal.

#### **IV. Tabular Material**

##### Projects Completed 2003-2004

720/4/93	Exposure Assessment and Decision Rules in Compliance Testing for Implementation of Exposure Limits. Published.
700/2/98	Natural and Unnatural Substances Related to Human Health. Published in <u>PAC</u> with follow-up summary in <u>CI</u> which then prompted several lay press publications.
2000-034-2-700	Glossary for Toxicokinetics of Chemicals. Undergoing publication.
2000-059-1-700	Properties and Units for Transfusion Medicine and Immunohaematology. Published.

2001-077-2-700 Best Practices for Workplace Exposure Assessment: A Critical Review of Methodology. **Abandoned.**

Current Projects (all end in -700)

- 1999-047-1- Immunochemistry of Metal Sensitization.
- 2000-009-1- Drug Metabolism Terms.
- 2000-010-1- Human Drug Metabolism Database.
- 2000-014-1- Recommendations for the Use of Nanotechnology in Clinical Laboratories.
- 2001-048-2- Research and Training in Medicinal Chemistry in India, Pakistan and Sri Lanka.
- 2001-049-2- Glossary of Terms Used in Process Chemistry/Manufacturing of Active Pharmaceutical Ingredients, and Pharmaceutics.
- 2001-050-2- Chemical, Pharmacological Aspects of Natural Products with Medicinal and Nutritive Value.
- 2001-053-2- Fundamental Toxicology for Chemists.\*
- 2001-058-1- Concepts and Structure for Requests in Clinical Laboratories.
- 2001-066-1- Global Use of the C-NPU Concept System for Properties in Toxicology.
- 2001-067-1- Properties and Units for Function Examinations.
- 2001-068-1- Properties and Units in Medical Molecular Biology.
- 2001-070-1- Properties and Units for Urinary Calculi.
- 2001-001-1- Compendium of Terms Associated With Drug Discovery and Development.
- 2002-051-1- Analogue-Based Drug Discovery.
- 2003-001-2- Explanatory Dictionary of Concepts in Toxicokinetics.
- 2003-028-1- Glossary for Chemists of Terms Used in Toxicology: Revision and Updating.
- 2003-044-1- Glossary of Terms Used in Combinatorial Chemistry.

- 2003-059-1- Quantifying the Effects of Compound Combinations.
- 2004-019-3- Glossary of Terms Used in Biomolecular Screening.
- 2004-023-1- Internationally Agreed Terminology for Observations in Scientific Communication.\*
- 2004-025-1- Compendium of Targets of the Top 100 Commercially Important Drugs.
- 2004-028-1- Practical Studies for Medicinal Chemistry: An Integrating Approach for Developing Countries.

\* Denotes Interdivisional Project. In this regard, Division VII also participates on projects 2001-005-1-300 (Post-genomic Chemistry) and 2001-020-1-300 (Glossary of Terms and Basic Protocols Used in Photodynamic Therapy).

#### Projects Undergoing Review

- 2001-069-1- C-NPU Concepts and Traceability of Measurements.
- 2003-016-1- Integrating Environmental Exposure Pathways for Medicinal Products.\*
- 2004-020-1- Molecular Gastronomy.\*

\* Denotes potential Interdivisional Project.