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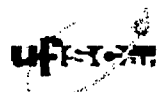
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UNITED NATIONS INDUSTRIAL
DEVELOPMENT ORGANISATION



INTERNATIONAL CENTRE FOR
SCIENCE AND HIGH TECHNOLOGY



DEPARTMENT OF CHEMISTRY
FEDERAL UNIVERSITY OF SÃO CARLOS

FINAL REPORT

Workshop on
*“Trends and Applications of Combinatorial Chemistry and
Combinatorial Technologies”*

20–23 November 2002
Hotel Fonte Colina Verde, São Pedro, SP - Brazil

UNIDO PROJECT TF/GLO/00/105
CONTRACT No.: 2002/250

OBJECTIVES

Following the recommendations of the steering committee of ICS-UNIDO an event had been organized in co-operation with the Department of Chemistry of the Federal University of São Carlos, SP – Brazil, in November 20–23, 2002.

This meeting was addressed to participants from academy, industry and R&D institutions from Latin American countries. The main objectives of the workshop were:

- To evaluate the state of the art of combinatorial chemistry and combinatorial technology and their industrial applications in Latin American.
- To introduce the combination of combinatorial chemistry and modern molecular biology
- To build awareness among industry and academic partners on a very rapid development of combinatorial chemistry and its relevance for industry in the region.
- To identify regional R&D institutions in South America through contacts established with the participants in the workshop.
- To give ICS an opportunity of identifying qualified countries to be considered as future co-operative institution for the ICS network.
- To evaluate possible initiatives (as follow-up projects and feasibility studies) of industry and academy concerning combinatorial chemistry from Latin American countries.
- To set up a regional ICS-UNIDO network on Combinatorial Chemistry and Combinatorial Technology.

ORGANIZATION

The workshop was organized jointly by the International Center for Science and High Technology (ICS), United Nations Industrial Development Organization (UNIDO) and Department of Chemistry, Federal University of São Carlos, SP-Brazil.

The local Organizing Committee was composed by Prof. Arlene G. Corrêa (Federal University of São Carlos, Brazil), Prof. Quézia B. Cass (Federal University of São Carlos, Brazil), Prof. Marcus Mandolesi Sá (Federal University of Santa Catarina, Brazil), Prof. Henning Ulrich

(University of São Paulo, Brazil), Prof. Vera Lucia Eifler Lima (Federal University of Rio Grande do Sul, Brazil), Prof. Edson L. S. Lima (Federal University of Rio de Janeiro, Brazil).

DATES AND VENUE

The workshop was held on 20-23 November 2002 at Hotel Fonte Colina Verde located in the city of São Pedro, SP-Brazil.

FUNDING

The expenditure sanctioned by UNIDO for this project was USD 17,500. The amount received from UNIDO on 5th November 2002 was USD 14,000 to cover the expenses towards the items listed in the budget. The hosting country (Brazil) contributed with USD 2,492 through various items. The Organizing Committee had covered tickets for all international participants and Brazilian participants living outside of São Paulo State. The arrangements for meals, hotel, etc., with reasonable costs and quality were made. A summary of the final budget is given in Appendix 1.

SCIENTIFIC PROGRAM

9 keynote one-hour lectures, 4 oral 30-min presentations, and 5 country/institution reports were presented during the workshop. The detailed workshop program is given in Appendix 2.

The key topics covered during the workshop were:

Thinking Combinatorially

- The Way to Molecular Diversity
- The Value of Combinatorial Technology

Chemical Synthesis of Libraries

- Split-Mix vs Parallel Synthesis
- Solid Phase vs. Liquid Phase Strategies; Resins & Scavengers
- Lab Automation, Miniaturization Technologies & Robotics

Characterization of Libraries

- Separation and Purification Methods (HPLC)

Drug Discovery

- Array-Based Libraries: Lead Discovery
- Focussed Libraries: Lead Optimization

High-Throughput Screening

- High-Throughput Medicinal Chemistry
- Ultra HTS

Materials Science

- Novel Catalysts

Informatics, Chemoinformatics, Bioinformatics

- Integration of Informatics with CombiChem
- Data Bases & Data Management

PARTICIPATION

Several forms and invitation letters were disseminated among most of the academic institutions, R&D institutes and industrial companies in order to acquire attendance of several lecturers and participants from the following countries: Argentina, Uruguay, Venezuela, Mexico and Chile. 55 participants and lecturers from 7 different countries including Argentina, Mexico, United States, Canada, Germany, Italy and Brazil took part in this workshop. Participants' affiliations included universities (81,8 %), R&D centers (9,1 %) and industry (9,1 %). Distribution of the participants according to countries is shown in Table 1.

Table 1. Participants according to countries

No.	COUNTRY	NUMBER OF PARTICIPANTS
1	Argentina	2
2	Mexico	1
3	Germany	1
4	USA	1
5	Italy	1
6	Canada	1
7	Brazil	48
	Total	55

Lists of lecturers and speakers of 30-min oral presentations from different countries are given in Tables 2 and 3, respectively. The complete lists of participants and lecturers are attached (Appendix 3).

Table 2. List of lecturers of the workshop

No.	KEYNOTE LECTURER	INSTITUTION	COUNTRY
1	Giorgio Fassina	Xeptagen	Italy
2	Ernesto G. Mata	National University of Rosário	Argentina
3	Paul Wentworth	Scripps Research Institute	USA
4	Luiz Juliano	Federal Univ. of São Paulo	Brazil
5	Jose M. Dominguez	Instituto Mexicano del Petroleo	Mexico
6	Aubrey Mendonca	Polymer Laboratories	Canada
7	Eliezer Barreiro	Federal Univ. of Rio de Janeiro	Brazil
8	Glaucius Oliva	University of São Paulo	Brazil
9	Pierfausto Seneci	Nucleotide Analog Pharma AG	Germany

Table 3. List of speakers of short-presentations (30 min) and country report (20 min)

No.	SPEAKER	INSTITUTION	COUNTRY
1	Henning Ulrich	University of São Paulo	Brazil
2	Quezia B. Cass	Federal Univ. of São Carlos	Brazil
3	Vera L. E. Lima	Federal Univ. of Rio Grande do Sul	Brazil
5	Renata X. Kover	Extracta Mol. Naturais	Brazil
6	Adolfo Iribarren	INGEBI- CONICET-Univ. Buenos Aires	Argentina
7	Izaque A. Maia	CenPRA	Brazil
8	Saul G. Jacchieri	Fundação Antônio Prudente	Brazil
9	Marcus M. Sá	Federal Univ. of Santa Catarina	Brazil
10	Carlos A. Montanari	Federal Univ. of Minas Gerais	Brazil

WORKSHOP MATERIALS

Each participant and lecturer was provided with a workshop bag containing the following:

- Detailed workshop program
- List of participants with their mailing addresses
- Pen and notebook
- Identification badge

OPENING CEREMONY

The Opening Ceremony of the workshop was organized at the Conference Hall of Hotel Fonte Colina Verde. The function was presided over by Associate Professor Romeu C. Rocha Filho, dean of the Federal University of São Carlos. The other members of the table to welcome the participants were: Associate Professor Paulo Cezar Vieira, president of the Brazilian Chemical Society; Dr. Giorgio Fassina, ICS-UNIDO representative; and Dr. Arlene G. Corrêa, local organizer of the workshop.

SOCIAL EVENTS

Lunches and dinners were organized for all participants of the workshop. A welcome reception was given on the first evening of the workshop. An excursion was organized to the Federal University of São Carlos and historical Pinhal coffee-farm. A banquet followed by a party with live music was organized for all participants after the closing ceremony.

ASSESSMENT

Assessment of the workshop was performed by an optional questionnaire to all participants. A summary of this assessment is given in Table 4. According to the result of this assessment the workshop was very successful and the organization was excellent, most evaluations ranged from very good to excellent. All participants would recommend others to attend a similar activity.

Table 4. Summary of the questionnaire (%) based on 55 participants**A. Organization**

Item	Excellent	Very good	Good	Fair	No answer
2. Information process	34,6	34,6	26,9	3,9	-
3. Announcement and pre-course material	27,0	19,2	34,6	3,9	15,3
4. Scientific program	53,9	26,9	7,7	-	11,5
4.1 Applied lecture/workshop	50,0	42,3	7,7	-	-
4.2 Small working groups	7,7	19,2	23,1	11,5	38,5
4.3 Case studies	3,9	30,8	11,5	11,5	42,3
4.4 Time spent by lecturers in class and after class on specific questions	30,8	30,8	19,2	3,9	15,3

Item	Balanced	Unbalanced	No answer
4.5 students scientific knowledge	61,6	19,2	19,2

B. Duration of Program

Item	Just right	Too long	Too short	No answer
1. Number of days	96,2	3,8	-	-
2. Length of working days	96,2	3,8	-	-

C. Training facilities & hotel

Item	Excellent	Very good	Good	Fair	No answer
1. Lecture/Training rooms	57,8	26,9	11,5	-	3,8
2. Breaks/refreshments	42,3	34,6	23,1	-	-
3. Hotel accommodation	38,5	46,2	15,3	-	-
4. Meals at the hotel	30,8	34,6	30,8	3,8	-

D. Organizer's response

Excellent	Very good	Good	Fair	No answer
80,8	19,2		-	-

E. Overall program organization

Excellent	Very good	Good	Fair	No answer
65,4	30,8	3,8	-	-

F. Would you recommend to others to attend a similar activity in the future?

Yes	Maybe	No	No answer
96,2	3,8	-	-

G. Evaluation of lecturers and speakers

Item	Excellent	Very good	Good	Fair	No answer
1. Course Material	42,3	30,8	15,4	7,7	3,8
2. Resident lecture presentation	38,5	53,8	7,7	-	2,8
3. International lecture presentation	57,7	34,6	7,7	-	-
4. Ability of lecturers to answer specific questions	46,2	42,3	11,5	-	-

POSSIBLE FOLLOW-UP

In the concluding session, four workgroups were formed in order to discuss specific themes. The following conclusions were drawn in each group:

Group 1: Regional Needs

Coordinator: Dr. A. Iribarren

- Drug/Diagnostics: Brazil and also Argentina have interest in carry out more research in both fields of Medicinal Chemistry. Centers need to be implanted that develop the use of compounds from natural resources and combinatorial synthesis for drug discovery.

- **Chemistry/Biotechnology:** There are good professionals available for doing research on Chemistry and Biochemistry, but they need more training in combichem. The available positions for researchers are currently limited due to governmental funding politics. Interaction between industry and university science needs to be fostered, therefore it would be desired that science is conducted by industry in Brazil.
- **Natural/Synthetic:** Natural diversity in South America is unique and its concise exploitation should be improved in a more self-sustainable way. Many local research groups search for the synthesis of active compounds, but due to complex taxes and regulations the importation of reagents and equipment is restricted. For effective collaborations and developing science in Brazil, it would be necessary to change customs' procedures in order to ease importation of reagents.
- **Patenting/Regulations:** Low partnerships between academia and industry; researchers need more information and specialized assistance.

Group 2: Training Needs

Coordinator: Dr. P. Seneci

- Not a major need, compared to other previous follow-up events where Dr. Seneci has participated.
- **Fellowships:** major need for young students in areas such as synthetic and molecular modeling CombiChem, HTS, analytical techniques in CombiChem
- **Training packages/ publication (important for teachers/academy)**
- **Websites:** useful for technical hints (supplies, reagents, new instruments)
- **Focal point training:** exchange information, accountability and assistance and reverse that to local needs. (in principle it is the person that organized the workshop – if for some reason the person can not do it we need to select a person for this position)
- **ICS consultancy:** important, especially to prepare projects in collaboration with industry.
- **ICS events:** not a first priority but some follow up events 2 or 3 years after this one is suggested.
- **Suggest to ICS UNIDO to create a start up laboratory for training researchers seeking for initiation in the field.**

Group 3: Networking Needs

Coordinator: Dr. A. Mendonca

- Networking & information transfer and distance between cities: forming a network internally with nodes and having a person responsible. Information can be transferred via e-mail. A homepage containing a databank of the combichem activities in the region is going to be implemented.
- Time factor for professors/less graduate student time: ICS-UNIDO could help to fund PDF's to lessen load on professors
- Access to decreased funding: ICS-UNIDO could help with some funding to supplement internal funding, as for example, via bilateral agreements, row funding, etc.
- Industry not used to carry out research/Regional funding: more awareness within the industry through nodes.
- Low partnerships between academia & industry: awareness maybe through external collaborations.
- Funding to transfer information: use financial support from external sources that UNIDO could help in sourcing.

Group 4: Project Needs

Coordinator: Dr. G. Oliva

- Identification: "Drug Discovery in Tropical and Endemic Diseases", a network of academic & industrial partners towards the discovery of new lead compounds against tropical and endemic diseases.
- Technology transfer: a professional evaluation of the economic impact of tropical and endemic diseases to help prioritize targets; consultancy in target reselection; design of high-throughput assays; partnership in screening; hits been passed to associated groups to expand via combichem; support in proper medicinal chemistry & pharmaceutical design; training in IP protection.
- Funding: fellowship for pos-doc/visiting professor to help; support the presentation of portfolio of projects to potential industrial partners.

CLOSING CEREMONY

Dr. G. Fassina and Dr. A. G. Corrêa expressed their satisfaction of the high scientific quality of presentations and activity of all participants.

APPENDIXES:

Appendix 1:

Budget Table and copy of bank demonstratives, tickets and receipts

Appendix 2:

Detailed program and list of lecturers and participants (with full addresses)

Appendix 3:

Advertisement of the workshop and hotel