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ICS-UNIDO
In cooperation with
National Institute of Chemistry
Slovenian Academy of Sciences and Arts

FINAL REPORT ON

*Meeting of Decision Makers from Academia, Chemical and Pharmaceutical
Industry on the Relevance of Combinatorial Chemistry
and Molecular Modeling,
July 1-2, 2000, Bled, Slovenia*

and

*Training Course on Molecular Modeling and
Computer Assisted Combinatorial Chemistry
July 3-7, 2000, Ljubljana, Slovenia*

UNIDO Project TF/GLO/00/105

Contract No 2000/112 106

Objectives

The main objectives of the Meeting of Decision Makers from Academia, Chemical and Pharmaceutical Industry on the Relevance of Combinatorial Chemistry and Molecular Modeling (Meeting) and the Training Course on Molecular Modeling and Computer Assisted Combinatorial Chemistry (Course), were as follows:

To build awareness among experts from industry and academic institutions on the relevance of molecular modeling (MM) and combinatorial chemistry/combinatorial technology (CC/CT).

To identify the problems of chemical and pharmaceutical industry in Eastern and Central European countries.

To identify the academic and industrial institutions that are able to promote MM and CC/CT.

Organization

The Meeting of Decision Makers from Academia, Chemical and Pharmaceutical Industry on the Relevance of Combinatorial Chemistry and Molecular Modeling and Training Course on Molecular Modeling and Computer Assisted Combinatorial Chemistry were organized by the International Center for Science and High Technology (ICS), United Nations Industrial Development Organization (UNIDO), in cooperation with the National Institute of Chemistry (local organizer) and the Slovenian Academy of Sciences and Arts. Dates and Venue: July 1-2, 2000, Bled, Slovenia.

The Meeting of Decision Makers from Academia, Chemical and Pharmaceutical Industry on the Relevance of Combinatorial Chemistry and Molecular Modeling took place between July 1-2, 2000 in Bled, Slovenia.

The Training Course on Molecular Modeling and Computer Assisted Combinatorial Chemistry took place between July 3-7, 2000 at the National Institute of Chemistry in Ljubljana, Slovenia.

Funding

The ICS-UNIDO approved contribution for both events was of US\$ 30,000.

The amount received from UNIDO in April 2000 was US\$ 24,000.

The actual expenditure from the ICS-UNIDO contribution was of US\$ 25,945

The final balance is of US\$ 1,945, still due to the local organizers

The hosting country contributed US\$ 8,000.

The actual expenses from the UNIDO contribution were lower than the foreseen sum, mainly because of cheaper travel expenses of participants and due to the effort to make arrangements for lodging and meals at a reasonable price. The funds we are still expecting from the Vienna office do not amount to US\$ 6,000, but only US\$ 1,945.

A summary of the final budget is given in Appendix I.

Participation

At the Meeting 18 participants – decision-makers - took part, out of which 12 delivered lectures or presented contributions. For the list of speakers at the Meeting see the attached program.

At the Training course 22 trainees took part and 10 were lecturers. The participants (trainees) presented their country and institutional reports.

Materials

Each participant at the Meeting and at the Training course obtained a bag with all the essential informations concerning Slovenia, lecture notes, program, list of participants, pen, notebook and the badge.

Opening ceremony

At the Bled Meeting Professor Robert Blinc addressed the participants in behalf of the Slovenian Academy of Sciences and Arts.

At the opening ceremony of the Course Professor Jure Zupan, the head of the Scientific Council of the National Institute of Chemistry addressed the participants.

Programs

The programs of the meeting and the Course are given in the Appendix.

Social Events

Come Together Party was organized for the Participants of the Meeting on Friday June 30 at 8 pm.

Assesment of the Workshop

Assessment was performed by the questionnaire distributed to the participants. The results are summarized in the table below.

ITEM	Excelent	Very good	Good	Fair	Poor
Announcement	20 %	49 %	24 %	7 %	
Scientific Program	26	55	19	0	
Lecture Room	62	38	0	0	
Breaks/refreshments	42	32	21	5	
Hotel	45	36	19	0	

Organizer's response	67	28	5	0
Course Material	26	38	26	10
Local speakers	50	40	10	0
International speakers	47	53	0	0

According to the filled questionnaires about one half of the participants would like to have more case studies, while the other half would like to have more practical sessions devoted to molecular modeling. Therefore one obtains the impression that the program was relatively well balanced.

Some participants proposed to have more lectures devoted to the biological applications. More participants proposed that the lecturers would provide their materials in the electronic form (ftp,html,CD-ROM) rather than that they carry back home large quantities of paper.

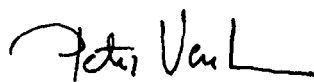
Conclusions


Both events turned out to be very useful both for the industrial as well as the academic communities of the Eastern and Central European countries. The participants became aware of the tremendous importance of combinatorial technologies and molecular modeling for the future of the chemical and pharmaceutical industry. The important take home message of both events is that the research pharmaceutical companies on long terms will not survive without the introduction of the two important groups of the methods.

The Decision-Makers' meeting led to preliminary proposals of follow-up activities, mainly focused on the need of networking of CEE institutions and the setting-up of CC/CT institutions/laboratories in selected CEE countries.

Ljubljana, 9 August 2000


Dr. Janez Mavri


Dr. Peter Venturini,
Director of Research

 KEMIJSKI INŠTITUT, LJUBLJANA, SLOVENIJA
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Budget for the Meeting and the Course

	Planned in US\$	Realized
<u>Meeting of Decision Makers</u>		
ICS-UNIDO contribution in US\$ 10000		
Accommodation and meals for 6 invited international lecturers	2520	2380
Accommodation and meals for 4 lecturers from the country for 3 days	1680	1504
Travel of 6 invited international lecturers (average 700 US\$)	4800	2416
Travel of 4 lecturers from the country	200	227
Transport (airport-hotel-airport)	200	750
Conference Hall	800	-
Meeting material	600	1520
<i>Subtotal</i>	10000	8797
Contribution of the hosting institution (secretariat, fax, telephone)	400	-
Contribution of industries (with this funds we will be able to cover cost of about four participants)	4400	-
<i>Subtotal</i>	4400	
<i>Grand Total for the Meeting</i>	14400	8797
<u>Training Course on Molecular Modeling and Computer Assisted Combinatorial Chemistry</u>		
ICS-UNIDO contribution US\$ 20000		
Accommodation and meals for 5 invited international lecturers (full board for 6 days)	3000	3140
Meals for 2 lecturers from the country	400	-
Accommodation and meals for 20 invited participants (full board for 6 days)	9600	9149
Travel of 5 invited international lecturers (average air-fare 500 US\$)	2500	684
Travel of 15 international participants (average fare 260 USD)	3900	2876
Travel of 5 participants from the country (average ticket 60 USD)	300	1173
Transport (airport-hotel-airport)	300	126
<i>Subtotal</i>	20000	17148
Contribution of the hosting institution (hardware and software)	4200	4200
Secretariat	400	
Fax/telephone/post	1000	1000
Conference hall	2000	2000
Training materials	800	800
<i>Subtotal</i>	8400	8000
<i>Grand Total for the Workshop</i>	28400	25148
Grand Total for the Meeting plus the Workshop (ICS-UNIDO)	30000	25945
Grand Total for the Meeting plus the Workshop (Local)	12800	8000
Grand Total	42800	33945

**Meeting of Decision Makers from Academia, Chemical and Pharmaceutical
Industry on the Relevance of Combinatorial Chemistry and Molecular Modeling,
July 1,2, 2000, Bled, Slovenia**

Tentative Program

Friday, June 30

20:00 Come Together Party

Saturday, July 1

9:15 S.Miertus Inaugural Session (S.Miertus, R. Blinc, P.Venturini)
Introduction to ICS-UNIDO Program CC/CT.

Session I *Principles Methods and Industrial Application of CC/CT*
G. Fassina Introduction to CC.
P. Seneci Basic Principles of CC and HTS.
P. Seneci Industrial Application of CC/CT.
G. Fassina Economic and patenting in Combinatorial Technologies.
G. Fassina Application of Combinatorial Technologies in Biotechnology: a
Case Study.

14:00-16:00 Lunch Break

Session II *Role of Computational Chemistry and Molecular Design*
J. Tomasi Computational Chemistry :Progress done and Limits Remained.
J. Mavri Irreversible Inhibition of the HIV-1 Protease:Can we predict the
Specificity?
MSI speaker Industrial Application of Molecular Modeling.

Session III *From Structure to Function*
D. Turk Role of crystallography in inhibitor design
M. Čarman Kržan Pharmacology-challenges of the 21-st century

Sunday, July 4

Session IV *Situation in CEE Countries*
9:00-12:00
G Narray-Szabo Bridges between academy and industry in Central and
Eastern European countries: where is the bottle-neck?

M. Japelj, KRKA Situation in Slovenia
T. Šolmajer, LEK Structure based design of enzyme inhibitors:
Current challenges and future prospects.
PLIVA speaker Situation in Croatia

Koubek Situation in Czech Republic
V. Bales Situation in Slovakia
A.P. Mazurek Impact of molecular modelling on new drug development
and marketing authorization
J. Martifalvi Situation in Hungary

12:00 Coffee break

Session V

Perspectives and Follow-up

Presentation of possible method initiative

12:15-13:00

S. Miertus: ICS-UNIDO Network

13:00-14:00

J. Margitfalvi: Proposal for a Central European Center for
Combinatorial Chemistry and of a Network of Combinatorial
Chemistry

and Molecular Design 14:00-17:00

Lunch break

17:00-

Conclusion and Recommendation

Round Table Discussion and Possible Common Initiatives

**Meeting of Decision Makers from Academia, Chemical and
Pharmaceutical Industry on the Relevance of Combinatorial Chemistry
and Molecular Modeling,**

July 1-2, 2000, Bled, Slovenia



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**Program of the Training course on Molecular Modeling and
Computer Assisted Combinatorial Chemistry
July 3-7, 2000, Ljubljana, Slovenia**

Monday, July 3

- 8:30- 9:30 Registration
9:30-10:30 Introduction to Training Course
(S. Miertus)
10:30-11:00 Coffee Break
11:00-13:00 Combinatorial Chemistry and Combinatorial Technologies
(G. Fassina)
13:00-14:30 Lunch
14:30-15:45 Combinatorial Chemistry : Industrial Applications and Case Studies
(G. Fassina)
14:30-15:45 Structure Representation in QSAR Studies
(M. Novic)
15:45-16:00 Coffee Break
16:00-17:30 Introduction to Molecular Mechanics: Force Fields, Molecular Docking,
Minimization
(R. Millini)
17:30-18:00 Discussion

Tuesday, July 4

- 9:00-11:00 Molecular modeling (Visualization, model building,
molecular databases, sequence alignment, homology models)
(R. Jerala)
11:00-11:30 Coffee Break
11:30-13:00 Quantum Mechanics : Principles, Methods, Effects
of Environment (Solvent, Crystal Field)
(J. Mavri)
13:00-14:30 Lunch
14:30-16:00 Molecular Modeling Practical Session
(J. Mavri)
16:00-17:00 Discussion

Wednesday, July 5

- 9:00-12:00 Computational Aspects of Combinatorial Library Design
(V. Gillet)
12:00-12:15 Coffee Break
12:15-13:15 Computational Approach in Prediction of Toxicity
(M. Vracko)
13:15-14:30 Lunch
14:30-15:30 Quantum Mechanics/Molecular Mechanics
(J. Mavri)
15:30-16:30 Practical Session on Molecular Mechanics
(R. Millini)

16:30-16:45 Coffee Break
16:45-18:00 Practical Session on Quantum Mechanics
(J. Mavri)

Thursday, July 6

9:00-10:00 Molecular Dynamics, Monte Carlo, Free Energy Calculation
(J. Mavri)
10:00-11:15 Process Simulation
(M. Fermeglia)
11:15-11:30 Coffee break
11:30-13:00 Application of Molecular Modeling
Drug design (S. Miertus)
Catalysis (R. Millini)
13:00-14:30 Lunch
14:30-15:30 Practical Session on Molecular Dynamics
(J. Mavri)
15:30-15:45 Coffee Break
15:45-17:15 Practical Session on Process Simulation
(S. Fermeglia-Prigl)
17:15-18:00 Discussion

Friday, July 7

9:00-10:45 Country and Institutional Reports of the Participants
10:30-11:00 Coffee Break
11:00-12:00 Country and Institutional Reports of the Participants (Continued)
12:00-12:30 Closing Session
12:30 Lunch

**Training Course on
Molecular Modelling and Computer Assisted Combinatorial Chemistry
Ljubljana, Slovenia, July 3-7, 2000**

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**Training Course on
Molecular Modelling and Computer Assisted Combinatorial Chemistry
Ljubljana, Slovenia, July 3-7, 2000**

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