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**International Centre for Science and High Technology
United Nations Industrial Development Organization**

in cooperation with

Faculty of Science, Eötvös University

also supported by the Italian Embassy in Budapest

Final Report on

***Trends and Applications of Combinatorial Chemistry and
Combinatorial Technologies***

Budapest, Hungary, 15–18 October, 2001

UNIDO Project TF/GLO/00/105

Contract No. 2001/311/IR

OBJECTIVES

This meeting was addressed to participants from academia, industry and R&D institutions from Central–Eastern European countries. The main objectives of the Workshop were as follows:

- To evaluate the state of the art of combinatorial chemistry and combinatorial technology and their industrial applications in Central–Eastern Europe.
- To build awareness among industry and academic partners on the very rapid development of combinatorial chemistry and its relevance for industry in the region.
- To identify regional R&D institutions in Europe 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 Central–Eastern European countries.
- To set up a regional ICS-UNIDO network on Combinatorial Chemistry and Combinatorial Technology.

ORGANIZATION

The Workshop was jointly organized by the Faculty of Science, Eötvös University in the Hotel Aura which is located inside the campus of the Methodology and Information Centre for In-service Teacher Training of the Ministry of Education in Pilisborosjenő between 15–18 October, 2001.

Members of the scientific committee:

- Prof. Stanislav Miertus, ICS-UNIDO, Trieste, Italy
- Dr. Giorgio Fassina, Italy
- Dr. Pierfausto Seneci, Germany
- Prof. Gábor Dibó, Eötvös University, Hungary

Members of the local organising committee:

- Dr. Péter Arányi, Chinoïn-Sanofi, Hungary
- Dr. Ferenc Darvas, Comgenex, Hungary
- Prof. Gábor Dibó, Eötvös University, Hungary
- Dr. István Greiner, Gedeon Richter, Hungary
- Prof. István T. Horváth, Eötvös University, Hungary
- Dr. András Kotschy, Eötvös University, Hungary
- Dr. László Kovács, InFarmatik, Hungary
- Prof. Gábor Náray-Szabó, Ministry of Education, Hungary

The ICS-UNIDO`s approved contribution was US\$ 25,000.

The amount received from UNIDO on 11 October, 2001 was US\$ 20,000.

The actual expenditure from the ICS-UNIDO contribution was of US\$ 21,367

The final balance is of US\$ 1,367 still due to the local organizers

The hosting country contributed US\$ 10,000.

The actual expenses covered by the UNIDO were lower than the foreseen sum, mainly because of cheaper lodging and meals since the Ministry of Education provided its facilities at a significantly reduced price.

A summary of the final budget is given in *Appendix 1*.

LECTURERS

Dr. Wolfram Altenhofen	Chemical Computing Group	Germany
Dr. Péter Arányi	Chinoin-Sanofi, Co.,	Hungary
Dr. Wolfgang Bender	Bayer AG	Germany
Dr. György Dormán	Comgenex	Hungary
Prof. Alexey Eliseev	Therascope AG	Germany
Dr. Giorgio Fassina	Xeptagen SpA	Italy
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Prof. György Kéri	Semmelweis University	Hungary
Dr. László Kovács	Infarmatik Ltd.	Hungary
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Prof. Stanislav Miertus	ICS-UNIDO	Italy
Prof. Claude Mirodatos	CNRS 2	France
Prof. Béla Noszál	Semmelweis University	Hungary
Dr. Menotti Ruvo	Xeptagen SpA	Italy
Dr. Pierfausto Seneci	NAPAG	Germany
Dr. Peter Van Den Brink	Avantium Technologies BV	The Netherlands

See full list and addresses in Appendix 2.

PARTICIPATION

Participation was open to scientists, researchers, postgraduate students, government administrators, industrialists and managers involved in the field of combinatorial science or willing to introduce the adequate modern combinatorial technologies in their home countries. The total number of the registered participants was 78.

Country	Academia	Industry	Total
Brazil	2	0	2
Bulgaria	5	0	5
Croatia	0	5	5
Estonia	1	1	2
Germany	1	0	1
Hungary	20	19	39
Kazakhstan	1	0	1
Poland	1	0	1
Romania	7	1	8
Russia	4	0	4
Slovakia	3	0	3
Sweden	0	1	1
Switzerland	1	0	1
Ukraine	3	2	5
Total	49	29	78

See full list with addresses in Appendix 3.

MATERIALS

Each participant at the Workshop obtained a bag with all the essential information and map of Budapest, lecture notes, program, list of participants, pens, notebook and the badge.

OPENING CEREMONY

The Opening Ceremony was attended by ca. 100 people: invited guests, the lecturers and the participants. The opening ceremony was sponsored by the Bayer AG, Germany. The Opening ceremony was addressed by

- ◇ Stanislav Miertus, Area Director, ICS-UNIDO
- ◇ Gábor Szabó, Deputy State Secretary of Research and Development, Ministry of Education
- ◇ Norbert Kroó, General Secretary of the Hungarian Academy of Science
- ◇ Benito Righetti, Science & Technology Attache, Italian Embassy
- ◇ Ferenc Láng, Dean, Eötvös University, Faculty of Science
- ◇ Zoltán Vincze, Dean, Semmelweis University, School of Pharmacy

Other invited guests:

- ◇ Dana Vavrikova, Deputy Head, ITPO office of UNIDO
- ◇ Sándor Görög, Head of the Chemistry Branch of the Hungarian Academy of Science

PROGRAM

The programme of the Workshop is enclosed in *Appendix 4*.

SOCIAL EVENTS

The registration and informal visit to the Faculty of Science, Eötvös University was organized on October 14 (Sunday). The Opening Ceremony was followed by a Reception for all attendees on October 15 (Monday). A Farewell Banquette was held after Prof. Árpád Furka's Closing Lecture on October 18 (Thursday).

The Reception and the Banquette were generously sponsored by the Bayer AG, Germany.

ASSESSMENT OF THE WORKSHOP

A questionnaire was distributed to the participants. The results are summarized in the table below.

Item	Excellent %	Very good %	Good %	Fair %	No reply
The information process was	58	32	7	0	3
Announcement & pre-course material	37	44	15	0	4
Scientific program (general)	41	44	12	0	3
Lecture/workshop	41	44	15	0	0
Small working group	12	12	33	15	28
Case studies	12	44	24	5	15
Extra-time specific question/examples	29	34	29	3	5
Students	Balanced	Unbalanced	No reply		
Students scientific background	71	12	17		
Duration of programme	Just right	Too long	Too short		
Number of days	93	5	2		
Length of working day	45	50	5		
Training facilities	Excellent	Very good	Good	Fair	No reply
Lecture/training rooms	54	32	12	0	2
Breaks/refreshments	46	38	12	2	2
Hotel accommodation	55	22	12	2	9
Meals at the hotel	14	17	50	14	5
Organizer's response	67	26	5	0	2
Overall programme organization	36	48	12	0	4
Follow-up	Yes	Maybe	No		
Would you recommend to others	88	7	0		5

In summary, it is a great honour for the organizer to receive the student's feedback with such high appreciation; the overall score of the top two grades (excellent + very good) was 77%. Students found the following insufficiencies: more small working group activities and case studies are needed; the schedule was too tough (in spite of the fact that the after-dinner discussions were cancelled); the meals at the hotel were low graded.

CONCLUSIONS

The Workshop proved to be very useful both for the industrial and for the academic communities of Central–Eastern European countries. The number of the participants well exceeded the proposed number as shown below.

		Academia	Industry	Subtotal
Lecturers	Domestic	5 (3)	4 (3)	9 (6)
	International	2 (2)	4 (2)	6 (4)
UNIDO		1 (0)	3 (0)	4 (0)
Participants	Domestic	20 (5)	19 (5)	39 (10)
	International	29 (20)	10 (20)	39 (40)
Total		57 (30)	40 (30)	97 (60)*

**The numbers proposed in the Term of References are put into brackets.*

The distribution of the participants has been approaching the proposed ratio. The topics of the lectures covered a broad field of combinatorial science and technology. The participants became aware of the tremendous impact of combinatorial chemistry on (i) drug discovery (ii) materials science, (iii) agrochemistry (iv) biological screening and (v) instrumentation. The important take home message is that combinatorial chemistry and combinatorial technology have become a powerful tool of the chemical and biochemical research and development process for the new millenium.

PROPOSALS FOR POSSIBLE FOLLOW-UP ACTIVITIES

The Workshop led to preliminary proposals of follow-up activities, mainly focused on the need of networking Central–Eastern European institutions and setting-up CC & CT educational and research centers in the CEE region.

The proposal of the Eötvös University, Budapest for becoming the first such regional center was supported by the majority of the attendees. The key position of the Eötvös University can be further substantiated:

- it played a pioneering role in the conceptual development of combinatorial chemistry
- undergraduate combinatorial chemistry courses have been held since 1999
- postgraduate combinatorial chemistry courses are initiated
- the setting-up of combinatorial research lab has been in progress
- the First Symposium of the European Society for Combinatorial Science (Eurocombi-1) was held in the Congress Centre of the University on July 1–5, 2001
- the present Workshop was organized by the University.

Representatives of the Russian participants from Moscow also showed high interest to form another regional combinatorial chemistry and technology center. That might provide an important bridge between the European and Asian states in the future.

Prof. Pierfausto Seneci's remarks and recommendations are enclosed in *Appendix 5*.

Budapest, 18 November 2001.



Gábor Dibó, Ph.D.
Associate Professor
Eötvös University
local organizer

Appendix 1

FINAL BUDGET

*Trends and Applications of Combinatorial Chemistry and Combinatorial
Technologies*

Budapest, Hungary, 15–18 October, 2001

Trends and Applications of Combinatorial Chemistry and Combinatorial Technologies
 Budapest, Hungary, October 15-18, 2001
 CC/CT (1.4)

Rate of Exchange: 278 local currency(Hungarian forint HUF)/dollar

BUDGET UNIDO

TOTAL FUNDS FROM ICS-UNIDO US dollars 25,000
 TOTAL FUNDS FROM UNIDO HUF 6,975,000

DESCRIPTION	Budget in US\$	Budget local curr.	Disbursement US\$	Disbursement l.c.	Difference USD\$	Difference l.c.
Travel						
<i>International lecturers</i>	3,600	1,004,400	4,412	1,230,948	(812)	(226,548)
Dr. Altenhofen, Wolfram			320			
Prof. Eliseev, Alexey			322			
Dr. Mendonca, Aubrey			1,400			
Prof. Mirodatos, Claude			1,320			
Dr. Van den Brink, Peter			1,050			
			0			
<i>National lecturers</i>	300	83,700	0	0	300	83,700
<i>International participants</i>	4,000	1,116,000	6,711	1,872,369	(2,711)	(756,369)
Babaev, Eugene			414			
Bodis, Jeno			10			
			185			
Boroduk, Oleg			54			
Cascaval, Alexandru			39			
Dehelean, Gheorghe			53			
Dias, Dias La			94			
Dugovic, Branislav			21			
Enkvist, Erki			320			
Fisyuk, Alexander			460			
Furdik, Mikulas			18			
Handzik, Jaroslav			76			
Hutinec, Antun			71			
Ivanova, Gabriela			210			
Kakalik, Ivan			18			
Ketegenov, Tlek, A.			600			
Limbeck, Marcus			232			
Markova, Vary			208			
Money, Valentin			210			
Nikitin, Mikhail			500			
Novokshonov, Vladimir			404			
Rangelov, Miroslav			210			
Sa, Marcus Mandolesi			780			
Silveira, Gustavo Pozza			780			
Tatarov, Vasyl			55			
Tripsa, Josif			220			
Vayssilov, Georgi N.			380			
Winkler, Igor			89			
<i>Total travel</i>	7,900	2,204,100.00	11,123	3,103,317	(3,223)	(699,217)
Accommodation & meals						
<i>international lecturers meals (10)</i>			424	118,287		
Hotel Hyatt			177	49,439		
Hotel Liget	2,400	669,600	255	71,096		
Hotel Gellert			312	87,102		
Hotel Peregrinus			476	132,800		
<i>international participants hotel (39)</i>	8,000	2,232,000	3,479	970,400		
<i>international participants meals (39)</i>			1,653	461,318		
<i>national lecturers (9)</i>	1,800	502,200	382	106,457		
<i>national participants (39)</i>	2,000	558,000	1,653	461,318		
others	0	0	21	5,895		
<i>Total accommodation</i>	14,200	3,901,800	6,882	2,434,112	6,809	1,477,688
Local transportation	2,900	809,100	390	108,750	2,510	700,350
<i>Total local transportation</i>	2,900	809,100	390	108,750	2,510	700,350
Publications & proceedings	0	0				
Papers	0	0				
Editing	0	0				
<i>Total publications</i>	0	0	0	0	0	0
Miscellaneous	0	0				
Photocopying	0	0	622	173,600		
Rent of equipment	0	0				
Rent of premises	0	0	34	9,375		
Bank charges	0	0	160	44,840		
others (3)	0	0	206	57,474		
<i>Total Miscellaneous</i>	0	0	1022	285,689	-1022	-285,689
GRAND TOTAL	23,000	6,744,900	21,015	5,997,027	6,983	747,873
TOTAL BUDGET FROM UNIDO	23,000					
ALREADY TRANSFERRED AMOUNT (80%)	20,000					
REMAINING FUNDS TO BE TRANSFERRED (after actual disbursement)	1,337					

Appendix 2

LIST OF LECTURERS/ORGANIZERS

*Trends and Applications of Combinatorial Chemistry and Combinatorial
Technologies*

Budapest, Hungary, 15–18 October, 2001

ICS-UNIDO Workshop on „Trends and Applications of Combinatorial Chemistry and Combinatorial Technology”
Budapest, Hungary, October 15-18, 2001

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Budapest, Hungary, October 15-18, 2001

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Appendix 3

LIST OF PARTICIPANTS

*Trends and Applications of Combinatorial Chemistry and Combinatorial
Technologies*

Budapest, Hungary, 15–18 October, 2001

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Appendix 4

FINAL PROGRAMME

*Trends and Applications of Combinatorial Chemistry and Combinatorial
Technologies*

Budapest, Hungary, 15–18 October, 2001



**UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION
INTERNATIONAL CENTRE FOR SCIENCE AND HIGH
TECHNOLOGY, TRIESTE, ITALY**



EÖTVÖS UNIVERSITY, BUDAPEST



AMBASCIATA D'ITALIA BUDAPEST. HUNGARY

ICS-UNIDO Workshop on

**Trends and Applications of Combinatorial Chemistry and
Combinatorial Technologies**

Budapest, Hungary 15–18 October, 2001

Co-sponsors:

**Bayer AG, Germany
Lab-Comp Kft, Hungary
Merck Kft., Hungary
Chinoin Rt., Hungary
Spectrum-3D, Hungary
Mettler Toledo Kft., Hungary
Reanal Rt., Hungary**

SUNDAY

October 14, 2001

12:00 – 18:00 REGISTRATION

*Eötvös University, Faculty of Science
Chemistry Building, Gate 1/A
Pázmány Péter sétány 1/A
Budapest, H-1117*

**18:00 DEPARTURE FOR HOTEL AURA
(Symposium venue)**

*Methodology and Information Centre for In-service Teacher Training of
the Ministry of Education
Pilisborosjenő Fő út 1.
Pilisborosjenő, H-2097*

**19:00 HOTEL REGISTRATION
19:15 Dinner**

MONDAY

October 15, 2001

7:30 – 8:30 Breakfast

8:30 – 9:00 Stanislav MIERTUS (*ICS-UNIDO, Trieste, Italy*)
ICS-UNIDO Programmes – An Introduction

9:00 – 10:45 Giorgio FASSINA (*Xeptagen SpA, Naples, Italy*)
Combinatorial Technologies – An Overview

10:45 – 11:00 Coffee Break

11:00 – 12:45 Alexey ELISEEV (*State University of New York, Buffalo, NY, USA*)
Dynamic Combinatorial Libraries

12:45 – 13:15 Discussion

13:15 – 14:15 Lunch

14:15 – 16:15 Claude MIRODATOS (*CNRS, Villeurbanne, France*)
Combinatorial Optimization of Heterogenous Catalysis

16:15 – 16:30 Coffee Break

17:00 – WELCOME RECEPTION

In the Aula of the Methodology and Information Centre for In-service Teacher
Training of the Ministry of Education,
Pilisborosjenő, Fő út 1.

TUESDAY

October 16, 2001

7:30 – 8:30 **Breakfast**

8:30 – 9:30 **Wolfgang BENDER** (*Bayer AG, Wuppertal, Germany*)
The Bayer Synthon Concept

9:30 – 10:30 **Ferenc HUDECZ** (*Hungarian Academy of Sciences, Budapest, Hungary*)
Application of MS for Library Characterization

10:30 – 10:45 **Coffee Break**

10:45 – 11:45 **Giorgio FASSINA** (*Xeptagen SpA, Naples, Italy*)
Biological Methods for Library Characterization and Screening

11:45 – 12:45 **István T. HORVÁTH** (*Eötvös University, Budapest, Hungary*)
Application of Fluorous Biphasic Chemistry in Combinatorial Technology

12:45 – 13:15 **Discussion**

13:15 – 14:15 **Lunch**

14:15 – 15:15 **István GREINER** (*Richter Gedeon, Budapest, Hungary*)
Robotics & Lab Automation

15:15 – 16:15 **László KOVÁCS** (*InFarmatik, Budapest, Hungary*)
Combinatorial Process Research & Development

16:15 – 16:30 **Coffee Break**

16:30 – 18:30 **Wolfram ALTENHOFEN** (*Chemical Computing Group, Lörrach, Germany*)
QSAR Modelling to Library Design Strategies

18:30 – 19:30 **Dinner**

19:30 – **FREE TIME**

WEDNESDAY

October 17, 2001

- 7:30 – 8:30 **Breakfast**
- 8:30-9:30 **Memotti RUVO** (*Xeptagen SpA, Naples, Italy*)
Combinatorial Chemistry in Biotechnology - A Case Study
- 9:30-10:30 **Béla NOSZÁL** (*Semmelweis University, Budapest, Hungary*)
Combinatorial Phenomena in Biological Systems
- 10:30 – 10:45 **Coffee Break**
- 10:45-12:45 **Pierfausto SENECCI** (*NADAG, München, Germany*)
Molecular Diversity in Drug Discovery: A Critical Assessment
- 12:45 – 13:15 **Discussion**
- 13:15 – 14:15 **Lunch**
- 14:15 – 16:15 **Aubrey MENDONCA** (*Polymer Laboratories, Amherst, MA, USA*)
Solid Phase Synthesis – An Overview
- 16:15 – 16:30 **Coffee Break**
- 16:30 – 17:30 **Aubrey MENDONCA** (*Polymer Laboratories, Amherst, MA, USA*)
Solid Phase Synthesis – Recent Developments in Resin Technology
- 17:30 – 18:30 **Péter ARÁNYI** (*Chinoin-Sanofi, Budapest, Hungary*)
Role of Combinatorial Chemistry in Original Drug Discovery
- 18:30 – 19:30 **Dinner**
- 19:30 – **FREE TIME**

THURSDAY

October 18, 2001

7:30 – 8:30 Breakfast

8:30 – 10:15 Peter VAN DEN BRINK (*Avantium Technologies BV, Amsterdam, The Netherlands*)
High Throughput Technologies: An Exciting New Development in Process
Chemistry Research and Development

10:15 – 10:30 Coffee Break

10:30 – 12:30 György KÉRI (*Semmelweis University, Budapest, Hungary*)
Rational Drug Design and Signal Transduction Therapy
11:30 – 12:30

12:30 – 13:30 György DORMÁN (*ComGenex, Budapest, Hungary*)
Good Quality Libraries (Predicted and Measured Parameters)

13:30 – 14:15 Lunch

14:15 – 15:45 COUNTRY REPORT

15:45 – 16:00 Coffee Break

16:00 – 17:30 FOLLOW-UP SESSION

17:30 – 18:30 Árpád FURKA (*Eötvös University, Budapest, Hungary*)
Twenty Years in Combinatorial Chemistry

18:30 – BANQUETTE

Appendix 5

**Prof. Pierfausto Seneci's remarks &
recommendations**

*Trends and Applications of Combinatorial Chemistry and Combinatorial
Technologies*

Budapest, Hungary, 15–18 October, 2001

**Draft of ideas and proposals presented during the final session of the
Workshop on Combinatorial Chemistry and Technologies
15-18 October
Budapest, Hungary**

Representatives of 12 countries were attendees at the Workshop: Brazil, Bulgaria, Croatia, Estonia, Hungary, Kazakhstan, Poland, Romania, Russia, Slovakia, Ukraine. Each country presented a detailed Country Report, and each country committed to sending an electronic copy of it to ICS-UNIDO.

The Country Reports were the basis for the subsequent Follow-Up discussion, where several concrete proposals were advanced and discussed, with the help of Prof. Miertus and of ICS-UNIDO Scientific Consultants; the more preliminary, but nevertheless strong interest of other developing countries for the venue of introductory Workshops on CC/CT in their homeland was also expressed.

Among the major points for further actions, we may list:

- A proposal for the creation of a Regional (Central-East Europe) Centre for CC/CT in Budapest (Hungary), taking advantage of strong, existing academic and industrial competencies in the country. Responsible for further more detailed proposals: Dr. Dibo (Eotvos University), Dr. Dorman (ComGenex, Budapest) and Professor A. Furka (Eotvos University), S. Miertus (ICS-UNIDO Area Director), P.F. Seneci (ICS-UNIDO Scientific Advisor).
- A proposal from Russia to create a similar Regional (former soviet republics, central asian countries) Centre for CC/CT in Moscow (Russia), again taking advantage of the favorable mix of competencies and expertise in the city (both academic and industrial, especially in the field of chemical diversity generation). A first preliminary step will be for the defined local key contact (Prof. E. Babaev – Moscow University) to assemble a proposal draft for the creation of such a Centre and to send it to ICS-UNIDO; when such a document will be finalized, appropriate actions will be undertaken under the sponsorship and scientific consultancy of ICS-UNIDO and of its Scientific Advisors.
- Several countries showed a strong interest for a request coming originally from Croatia for a general ICS-UNIDO document containing guidelines for newcomers in the field of CC/CT. This document should contain pragmatic suggestions for academic and industrial institutions in developing countries to start simple activities in CC/CT; should specify the nature of simple, cheap „core modules” in terms of equipment and instrumentation necessary to start CC/CT activities; should provide useful contacts (scientific experts, ICS-UNIDO representatives, regional and national focal points in various developing countries, etc.) to be accessed for questions; in a word, should represent a comprehensive but practical indispensable tool for both newcomers in the field and for groups with little experience. A first draft of the proposal

should be prepared by Dr. Seneci by mid November, and a final document should be ready to be circulated (web, mail, etc.) to interested parties.

- Several countries showed a strong interest for a request coming originally from Croatia for a hands-on, practical Workshop on synthetic methodologies in CC/CT where attendees are introduced to experimental protocols in CC/CT (solid-phase synthesis, split-mix methods, parallel synthesis, analytical characterization and purification of libraries, and so on) through experiments performed in an equipped synthetic laboratory. As a candidate for the organization, Dr. Hutinec (PLIVA – Zagreb, Croatia) has expressed a possible interest of its company, well recognized in drug discovery and already possessing the necessary infrastructures (synthesis, automation and screening). Several other countries present during the Workshop expressed their interest in attending such a Workshop organized in Zagreb.
- Representatives from Bulgaria expressed the interest for more hands-on Training Courses based on computational techniques in CC/CT. As similar courses are already held twice a year in Trieste by ICS-UNIDO, the suggestion was taken as a strong need for their regular organization, maybe with even stronger hands-on components and with the invitation of experts in chemical diversity rational design and selection. The possibility of organizing dedicated hands-on Workshops in interested countries, e.g. Bulgaria, will also be considered if a strong interest will be confirmed in future.

Among more preliminary needs and interests expressed by attendees, we can list

- The interest expressed by Brazil to have a Workshop mostly devoted to the use of CC/CT in the search, isolation and rapid modification of natural products with biological activity for pharmaceutical purposes;
- The interest expressed by Poland to have more information about applications of CC/CT in catalysis and material science;
- The interest expressed by Kazakhstan to have more information about CC/CT in general via ICS-UNIDO sponsored initiatives (links or Workshops organized in the country);
- The strong motivation, provoked by the Workshop in Hungary via the excellent level of the Speakers, expressed by representatives from Slovakia, Ukraine, Romania and Estonia among others in pursuing the objective of introducing methodologies related to CC/CT in their projects and, via networking, in other groups in their countries.

As for general points related with the scientific levels of the presentations, a general consensus from attendees regarded both the quality of both Speakers and presentations, and the subjects chosen by the Workshop organizers. Among further topics to be considered, natural products and rational methods for chemical diversity selection and generation were mentioned.