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FINAL REPORT

"COMBINATORIAL CHEMISTRY AND MOLECULAR MODELING: METHODS AND INDUSTRIAL APPLICATIONS"

May 28 - Jun 2, 2000
Juriquilla, Querétaro.
México

UNIDO PROJECT
No. TF/GLO/00/105
Purchase ~Order No.: 05-0-32027

OBJECTIVES: The main objectives were:

- To promote Combinatorial Chemistry in México and in Latin América in general.
- To bring together all the researches from Mexico interested in the field.
- To discuss possibilities of a joint project of some Mexican institutions.
- To assist researchers from Instituto Mexicano del Petróleo in their training to use CC to develop new catalyst.
- To promote the use of Natural Products in CC/CT.
- To integrate México to the ICS-UNIDO network on CC/CT.
- To promote among graduate students CC/CT.
- To create contacts between CC/CT specialists and researchers from Latin American's countries.

ORGANIZATION:

This workshop was jointly organized by the Institute of Chemistry (UNAM), The local organizers were:
Dr. Juan Antonio Cogordan, (chair) Instituto de Química, UNAM
Dr. Manuel Salmón Salazar, Instituto de Química, UNAM
Dr. Raymundo Cea Olivares, Instituto de Química, UNAM
Dr. Raymundo Cruz Almanza, Instituto de Química, UNAM
Dr. Guillermo Delgado Lamas, Instituto de Química, UNAM
Dr. Ascensión Montoya, Instituto Mexicano del Petróleo

The scientific committee was formed with:

Professor Stanislav Miertus, ICS-UNIDO
Dr. Pierfausto Seneci, GlaxoWellcome, Italy.
Dr. Giorgio Fassina, Technogen, Italy

DATES:

The workshop was held at the hotel Mision Juriquilla, Querétaro. México from May 28 to June 2, 2000

FUNDING:

UNIDO-ICS

Co-funded by

UNIVERSIDAD NACIONAL AUTONOMA DE MEXICO
INSTITUTO MEXICANO DEL PETROLEO

A summary of the final budget is included in appendix 1.

The ICS-UNIDO contribution was of 30,000 USD and we received 24,000 USD (80%) according to the contract.
The actual expenses to be paid with UNIDO´s founds is of 26,911 USD and the balance (26,911-24000) of 2,911 USD plus the remaining 2,614 USD are consequently covered from local contributions, **thus NO additional transfer of money from UNIDO is required.**

LECTURES:

A total of 10 lectures from different institutions and countries participated in the workshop. as follows:

Lecturer	*Institution*	*Country*
Prof. Stanislav Miertus	ICS-UNIDO,	ITALY
Dr. Georgio Fassina	Tecnogen	ITALY
Dr. PF Seneci	Glaxo Wellcome	ITALY
Dr. Alex V Eliseev	U. of New Y. At Buffalo	USA
Dr. John Hewes	National Institute of Standards and Technology	USA
Dr. Gary Diamond	Symyx Technologies, Inc.	USA (Sta. Clara, California)
Dr. Antohony Volpe	Symyx Technologies, Inc.	USA (Sta. Clara, California)
Dr. Moises Hassan	Molecular Simulations, Inc.	USA (San Diego, Ca.)
Dr. Nina Pastor	Facultad de Ciencias UAEM	MÉXICO
Dr. Ignacio Rivero	Instituto Tecnológico de Tijuana	MÉXICO
Dr. Ernesto Mata	Instituto de Química Orgánica de Síntesis, Universidad de Rosario	ARGENTINA
Dr. Juan M. Dominguez	IMP	MÉXICO
Dr. Manuel Salmón	IQ-UNAM	MÉXICO
Dr. Hector Armendariz	IMP	MÉXICO

Dr. Ascensión Montoya IMP MÉXICO

PARTICIPANTS:

The workshop was intended for researchers from universities, research companies, government institutions and private enterprises. **The total number of participants (including lecturers) was of 35.**

COUNTRY	Number of Participants
Italy	2 Research institute
Italy	1 private enterprise
USA	4 Private enterprise
USA	1 Gov. institute
USA	1 Academy
ARGENTINA	1 Academy
MÉXICO	6 Research Institute
MÉXICO	2 Private enterprise
MÉXICO	17 Academy

Obs. : A large number of researchers and institutions from Latin American countries were contacted. Many of them did not answer. **Some of them confirmed their participation (such as Cuba and Costa Rica), but then did not show up.**

MATERIALS DISTRIBUTED:

A binding with a presentation of the workshop, the general program, schedule, abstracts and paper leaves to take notes was distributed, together with pens, pencils and a list of participants.

OPENING CEREMONY:

The opening ceremony was attended by Prof. S. Miertus, (ICS-UNIDO), Dr. J.M. Domínguez (Instituto Mexicano del Petróleo) and Dr. Manuel Salmón (Institute of Chemistry, UNAM).

MEETINGS:

The workshop arrangements were suitable for a diversity of meetings between the attendees. The exchange of information on academic issues was very important. The knowledge acquired by the researchers on the possible agencies for economical funding and scientific advice on CC/CT was valuable too.

WORKSHOPE PROGRAMME:

The workshop was organized in form to cover as many topics as possible of CC and CT. The lectures and discussions sessions from 9 to 20 hours, with lunch and coffee breaks. All the participants were interested in all the lectures, the . The response of the audience to the discussion sessions was a success, normally they lasted longer than the scheduled time. The availability and interest of the invited speakers was remarkable. The programme is given in Appendix 3.

SOCIAL, EDUCATIONAL AND CULTURAL ACTIVITIES:

To favor the exchange of information as much as possible, the organization of the workshop was planned to take full advantage of the hotel facilities. All the meals and breaks were held in common areas with the participation of all the attendees.
The following social events were attended by the lectures, participants and organizers during the workshop:

Additionally, a visit to the folkloric and colorful town of San Miguel de Allende on the afternoon of May 31st was arranged.

CLOSING CEREMONY:

Previous to the closing ceremony a general discussion with the participation of all the audience was carried out. To conclude, Professor Miertus made a summary of the workshop and he listed some of the possible actions to be taken for the future regarding CC and CT in the region. Finally Dr. Cogordan acknowledged to all the staff their enthusiastic assistance on all the practical arrangements. A special recognition was given to all the institutions involved in the financial support of the workshop.

ASSESSMENT:

Most of the participants ranged the workshop between very good and excellent. The results of the questionnaire, together with some plots, are shown in appendix 4.

RESULTS:

The workshop fulfilled its objectives.

The participation from Latin American countries was limited.

Appendix 1.

BUDGET

"COMBINATORIAL CHEMISTRY AND MOLECULAR MODELING: INDUSTRIAL APPLICATIONS"

Concept	ITEM	PROPOSED in USD	FINAL in USD
10 A & M Invited speakers	4 A & M invited speakers	8,400	♣3813
15 A & M Inter. particio	2 International particip.	9,450	♣2133
Travel of national participants and lectures	Travel of national participants and lecturers	5500	♣460
Travel of 25 international participants and lecturers	Travel 4 international	12,150	♣5124
Accomodation and meals for 20 participants from the country	Accomodation and meals for 20 participants from the country	10,500	♣10500
Accomodation and meals for 4 lecturers	Accomodation and meals for 4 lecturers	2,800	♣2800
Local transportation		1200	♣2081
Printed Mater			521
Advertising News Paper			672
Office Material			674
TEL. + FAX + POST			247
Secretarial Expenses			500
			29,525

♣ All these expenses were covered with UNIDO´s founds.

CONTRIBUTIONS	PROJECTED US DOLLARS	FINAL US DOLLARS
UNIDO	30,000	24,000
OTHER SOURCES	20,000	7,411
TOTAL	50,000	31,411

OBSERVATION:

The remaining 6,000 US Dlls in the contract will not be required.

Appendix 2.
List of Participants

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Appendix 3. Programme

ORAL PRESENTATIONS

Monday, May 29

TIME	AUTHORS	TITLE
8:30-8:40	**OPENING**	**CEREMONY**
8:40-9:05	S. Miertus	ICS-UNIDO Program
9:05-9:30	J.M. Domínguez	IMP
9:30-9:55	M. Salmón	IQ-UNAM
10:00-11:00	P.F. Seneci	Combinatorial Chemistry and Combinatorial Technologies: An Overview
11:00-11:20	**COFFEE**	**BREAK**
11:20-12:20	Alex V. Eliseev	Dynamic Combinatorial Chemistry
12:20:-13:20	P.F. Seneci	Combinatorial Synthetic Libraries: Design and Formats
13:20-13:40	Participants	Discussion session
13:40-16:30	**LUNCH**	**BREAK**
16:30-17:30	N. Pastor	Specificity in Protein-DNA Interactions explored with Molecular Dynamic Simulations
17:30-17:50		PHARMACY
17:50-18:10	COFFEE	BREAK
18:10-20:00	DISCUSSION	
20:00-22:00	DINNER	

ORAL PRESENTATIONS

Tuesday, May 30

TIME	AUTHORS	TITLE
9:00-10:00	P.F. Seneci	Purification and Quality Control of Synthetic Libraries
10:00-11:00	G. Fassina	Biological methods for the generation of combinatorial Libraries
11:00-11:20	COFFEE	BREAK
11:20-12:20	P.F. Seneci	Application of Combinatorial Chemistry to Catalysis
12:20-13:20	J. Hewes	Combinatorial Methods at the NIST
13:20-13:40	Participants	Discussion Session
14:00-16:00	LUNCH	BREAK
16:30-17:30	P.F. Seneci	Homogeneous Catalysis
17:30-17_50		NEW MATERIALS
17:50-18:10	COFEE	BREAK
18:10-20:00	DISCUSSION	
20:00-22:00	DINNER	

ORAL PRESENTATIONS

Wednesday, May 31

TIME	AUTHORS	TITLE
9:00-10:00	Gary Diamond	High Throughput Techniques for the Discovery of New Olefin Plymerization Catalysts
10:00-11:00	G. Fassina	LTS, MTS and HTS: Implications for Drug Discovery
11:00-11:209:05-9:30	COFFEE	BREAK
11:20	SIGHTSEEING	

ORAL PRESENTATIONS

Thursday, June 1

TIME	AUTHORS	TITLE
9:00-10:00	Anthony Volpe	Combinatorial Approaches to Catalysis Research
10:00-11:00	Moises Hassan	Diversity with Restraint. Design of Diverse, Drug-Like Libraries
11:00-11:20	COFFEE	BREAK
11:20-12:20	S. Miertus	Computer aided, drug design and combinatorial chemistry: case study of new HIV-1 PR inhibitors
12:20-13:20	G. Fassina	Application of combinatorial technologies in biotechnology: a case study.
13:20-13:40	Participants	Discussion Session
13:40-16:30	LUNCH	BREAK
16:30-17:30	Moises Hassan	Computer session
17:30-17_50		BIOTECHNOLOGY
17:50-18:10	COFEE	BREAK
18:10-20:00	DISCUSSION	
20:00-22:00	DINNER	

ORAL PRESENTATIONS

Friday, June 2

TIME	AUTHORS	TITLE
9:00-10:00	Ignacio Rivero	Organic Synthesis in Solid Phase (OSSP) and its Analytical Applications
10:00-11:00	Ernesto Mata	Solid-phase Organic Synthesis for the Development of Combinatorial Libraries
11:00-11:20	COFFEE	BREAK
11:20-12:20	G. Fassina	Economic and Patenting in Combinatorial Technologies
12:20-13:20	MEETING	EVALUATION
13:20-13:40	CLOSING	CEREMONY
13:40-16:30	LUNCH DEPARTURE	BREAK

Appendix 4.

Summary of the Questionnaire Results

Report

A Organization

1 How did you obtain information about this workshop?

QUESTION	%POSTER	%INSTITUTION	%ORGANIZER	%ICS	%INVITATION
1	25	30	10	5	35

2 The information process was.
3.- The announcement and pre-corse material was
4.- I found the scientific programme.
4.1.- Applied lecture/workshop
4.2.- Use of small working groups
4.3.- Case studies
4.4 The time spent by lectures in classs and after class on specific questions/examples

QUESTION	%EXCELLENT	%VERY GOOD	%GOOD	%FAIL	%NOT ANSWER
2	15	40	35	10	0
3	10	25	35	30	0
4	45	45	10	0	0
4.1	35	50	15	0	0
4.2	25	45	20	5	5
4.3	30	50	20	0	0
4.4	25	60	10	0	5

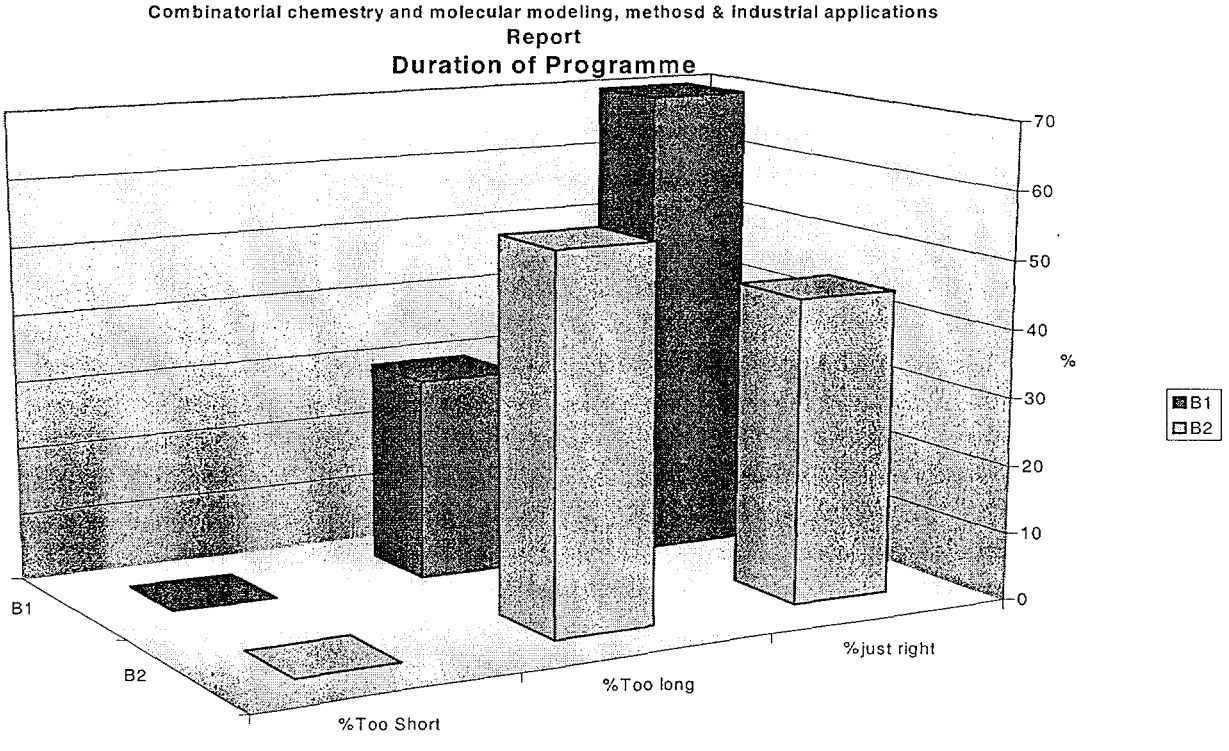
4.5 Students scientific knowledge was.

QUESTION	%BALANCED	%UNBALANCED	%NOT ANSWER
4.5	70	20	10

B Duration of Programme

B1 Number of days
B2 Lenght of working days

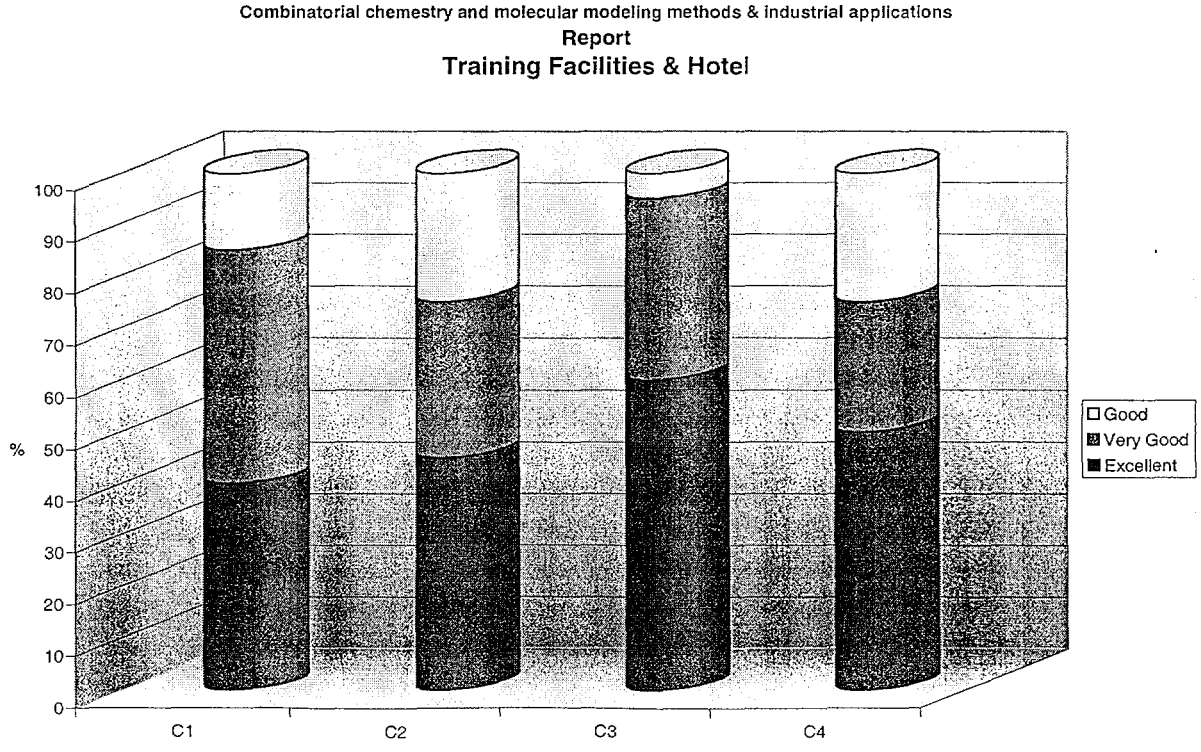
QUESTION	%JUST RIGHT	%TOO LONG	%TOO SHORT
1	70	30	0
2	45	55	0



C Training Facilities & Hotel

C1 Lecture/Trainig rooms
C2 Breaks/refreshments
C3 Hotel/accommodation
C4 Meals at the hotel

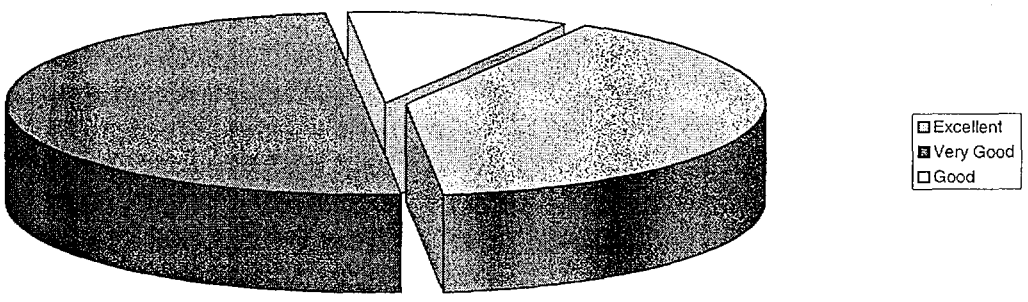
QUESTION	EXCELLENT	VERY GOOD	GOOD	FAIR
C1	40	45	15	0
C2	45	30	25	0
C3	60	35	5	0
C4	50	25	25	0



D Organizer´s responseto participants needs

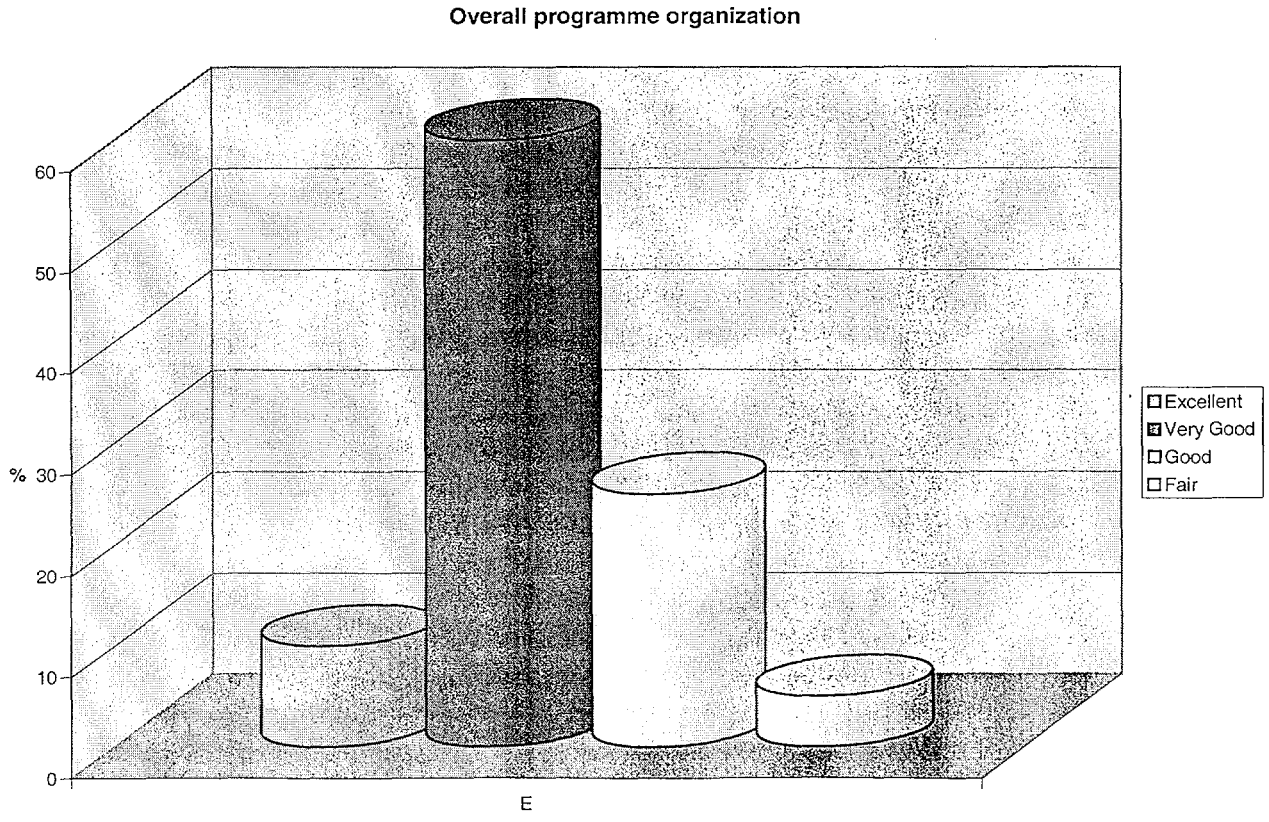
QUESTION	EXCELLENT	VERY GOOD	GOOD	FAIR
D	40	50	10	0

Combinatorial chemestry and molecular modeling methods & industrial applications
Report
Organizer response to participants needs



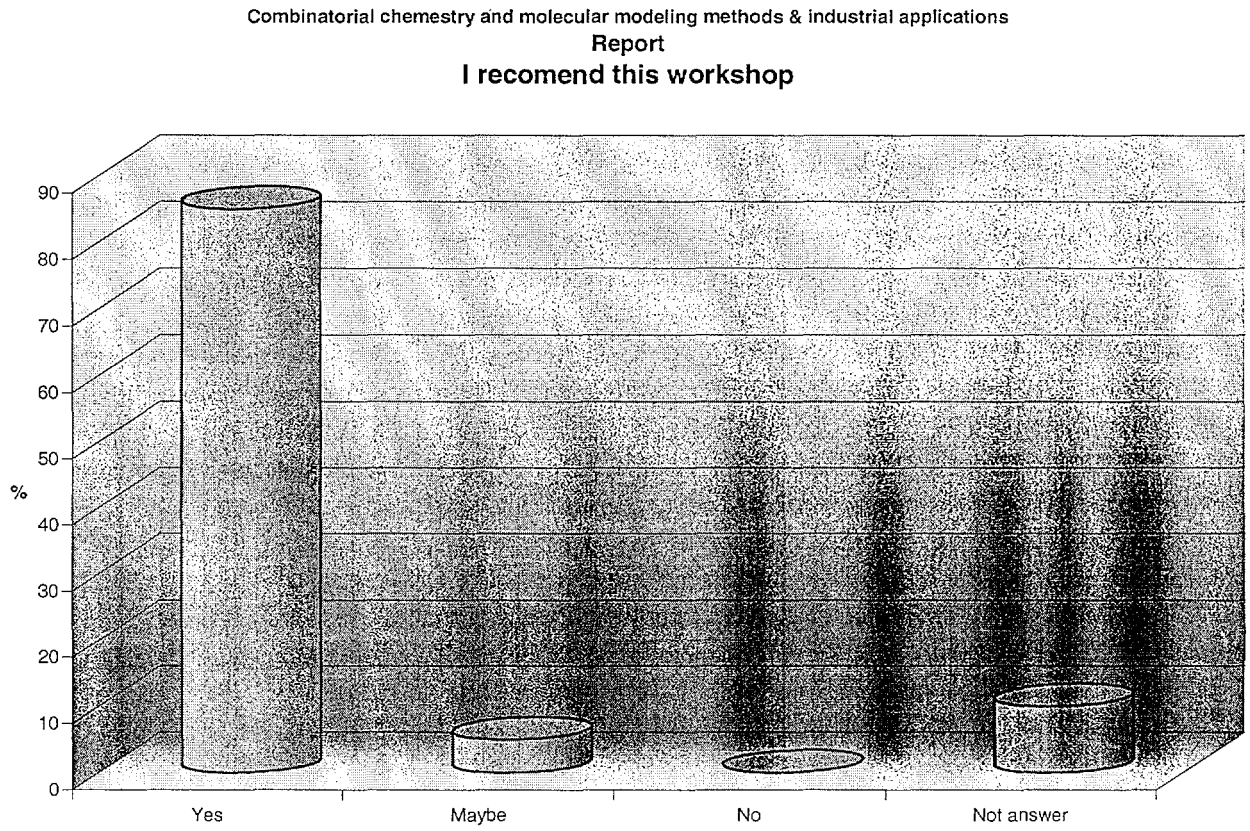
E. Overall program organization

QUESTION	EXCELLENT	VERY GOOD	GOOD	FAIR
E	10	60	25	5



F Would you recommend to other from your institution/contry to attend a similar activity in the future?

QUESTION	YES	MAYBE	NO	NOT ANSWER
F	85	5	0	10



G Evaluation of lectures and speakers

G1 Course material
G2 Resident lecture presentation
G3 International lecture presentation
G4 Ability or lecturers to anwer specific questions

QUESTION	EXCELLENT	VERY GOOD	GOOD	FAIR	NOT ANSWER
G1	25	35	20	10	10
G2	10	60	20	5	5
G3	35	55	5	0	5
G4	40	50	5	0	5