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FINAL REPORT

"COMBINATORIAL CHEMISTRY AND COMBINATORIAL TECHNOLOGIES"

19-23 APRIL 1999 LOS BAÑOS, LAGUNA PHILIPPINES

UNIDO PROJECT No. TF/GLO/96/105
CONTRACT No. 99/086

Objectives

The major objectives of the workshop are as follows:

- to build awareness among researchers, technologists and academicians on the development of combinatorial chemistry and combinatorial technologies (CC/CT)
- to update the participants on the principles and industrial applications of CC/CT
- to evaluate possible initiatives (as follow-up projects and feasibility studies) of industry and academe in Southeast Asia regarding CC/CT development and industrial implementation with the focus on the application of CC/CT to natural products research and exploitation
- to set up a regional ICS-UNIDO network on Combinatorial Chemistry and Combinatorial Technologies

Organization

This workshop was jointly organized by the International Centre for Science and High Technology (ICS-UNIDO) and the Institute of Chemistry, University of the Philippines, Los Baños (IC-UPLB). The local organizers were:

- Dr. Norma N. Fajardo (Chair)
- Dr. Cleofe A. Calanasan (Head, Technical Committee)
- Mr. Roy Roberto L. Gerona (Head, Secretariat)
- Dr. Maxima E. Flavier (Head, Ways and Means Committee)
- Ms. Maria Cecilia D. de Mesa (Head, Publicity and Physical Arrangements Committee)

The scientific committee was composed of local and international scientists who advised organizers about the content of the scientific programme. This committee included the following:

- Prof. Stanislav Miertus (ICS-UNIDO, Italy)
- Dr. Pierfausto Seneci (GlaxoWellcome, Italy)
- Dr. Giorgio Fassina (Tecnogen, Italy)
- Dr. Cleofe A. Calanasan (IC-UPLB, Philippines)

Dates

The workshop was held at the Continuing Education Center, University of the Philippines at Los Baños (UPLB), Laguna, Philippines from 19-23 April 1999.

Funding

The total contribution from UNIDO was US\$30,000. The Institute of Chemistry, UPLB provided the manpower support, conference facilities, documentation services and communication expenses.

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

Lecturers

A total of 6 lecturers from different institutions and countries participated in the workshop. Another lecturer, Dr Andrea Missio from GlaxoWellcome Italy, was unable to attend due to ill health, so the papers he prepared were presented by Dr. Seneci.

Lecturer	Institution	Country
Prof. Stanislav Miertus	ICS-UNIDO	Italy
Dr. Plerfausto Seneci	GlaxoWellcome	Italy
Dr. Giorgio Fassina	TECNOGEN	Italy
Dr. Anneliese Appleton	Molecular Simulations P/L	Australia
Dr. Lucia Carrano	Biosearch	Italy

lana 40 and 40 a	GlaxoWellcome	United Kingdom
l lie besondenie i M van Ametariam	I GIZYOWAIIMA	I IIDITAA KIDAAAAN I
Dr. Franciscus T. M. van Amsterdam	1 CIGNOTACIONIC	I United Kirking

The lecturers who presented the state-of-the-art in combinatorial chemistry and technologies were mainly from industrial institutions. The lectures were supported by discussions on different case studies highlighting the applications of CC/CT. The economics and patenting issues regarding CC/CT were also covered.

The lecturers' accommodations, living expenses and airfare (except Prof. S. Miertus) were fully sponsored.

Participants

The workshop was intended for participants from universities, research institutions, government institutions, and private companies engaged in the eleochemical, agrochemical and pharmaceutical industries. Participants involved in R and D and industrial processes were given preference. Applications were solicited from institutions throughout the Southeast Asian region via mail, e-mail, fax and telephone calls. The local committee with the assistance of ICS selected the participants.

Twenty seven (27) participants out of the 28 selected attended the workshop. The lone invitee from Indonesia failed to attend. Details of the geographical and institutional distributions of the participants are presented below.

Country	Number of Participants	
Hongkong	1 (academe)	
India	1 (research institute)	
Malaysia	1 (academe)	
Philippines	18 (7 from industry, 2 from govt institutes, 1 from research institute, 8 from academe)	
Taiwan	1 (industry)	
Thailand	4 (1 from academe, 3 from govt institutes)	
Vietnam	1 (research institute)	

A complete list of participants is given in Appendix 2.

Materials Distributed

Lecturers and participants were provided with a workshop bag containing the souvenir program, note pads, pens, directory, Philippine map and computer diskettes. Copies of lecture materials were also given to each participant.

Opening Ceremony

The opening ceremony was attended by Prof. Stanislav Miertus (ICS-UNIDO Area Coordinator), the lecturers and participants. Invited guests to this ceremony included Dr. Francisco Peñalba (Vice Chancellor for Community Affairs, UPLB), Dr. Ma. Cristina D. Padolina (Chancellor, UP Open University), Dr. Carol Yorobe (Assistant Secretary, Dept of Science and Technology), Dr. Pacifico C. Payawal (Dean, College of Arts and Sciences, UPLB), Dr. Ernesto J. del Rosario (Director, IC, UPLB) and Engr. Jun Montes (Representative, SPIK, Chemical Industries Association of the Philippines).

Meetings

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On 21 April 1999, a meeting was held among Mr. Roberto di Virgilio (Commercial Attache of the Italian embassy), Prof. Stanislav Miertus, Dr. Lucia Carrano, Dr. Glorgio Fassina and Dr. Pierfausto Seneci. Mr. Di Virgilio showed interest in the joint programme between ICS-UNIDO and the Institute of Chemistry, UPLB, and expressed his support for the plan of a CC/CT network in the Southeast Asian Region.

Another meeting was held between Prof. S. Miertus and Ms. Betty Koreh (UNIDO Program Officer in the Philippines). The latter expressed her strong interest and support for any follow-up activities to the workshop.

Workshop Programme

The workshop was organized as lectures and discussions from 900 to 1830 HRS. The programme is given in Appendix 3.

Social, Educational and Cultural Activities

The following social events were attended by the lecturers, participants and organizers during the workshop:

A visit to the flower and garden show in the university after the lectures on 19 April Swimming in a local hot spring resort in the evening of 19 April

A banquet at the ANEST Tower on 21 April 1999 which featured Philippine folk dances A trip to nearby towns of Los Baños, Laguna in the afternoon of 23 April 1999

Prof. Miertus, Dr. van Amsterdam and Dr Fassina took a boat ride in Laguna lake, the biggest body of freshwater in the Philippines on 20 April. On the 24th of April, the lecturers and International participants also visited Tagaytay which overlooks Taal volcano, the smallest active volcano in the world.

Closing Ceremony

The round table discussion on future actions and closing ceremony were attended by Ms. Betty Koreh (UNIDO Program Officer), Prof. S. Miertus (ICS-UNIDO Area Coordinator), Dr. Ernesto J. del Rosario (IC-UPLB director) and Dr. Alan Feranii (Philippine Council for Health Research and Development, DOST representative).

Assessment

The workshop was assessed by the participants using the questionnaire provided by ICS-UNIDO. A summary of this evaluation is given in Appendix 4. The participants' evaluation of the overall programme organization is from very good to excellent. All the participants said that they benefited from the workshop and will recommend others to attend a similar activity in the future.

The participants opined that the lectures ranged from very good to excellent and the number of days spent was just right. The evaluation of the training facilities/accommodation and the food ranged from good to excellent.

Results

At the start of the workshop, most of the participants had little or no knowledge of combinatorial chemistry/combinatorial technologies. Based on the results of the evaluation, the participants felt that the workshop has enlightened them on what CC/CT is all about. They found all the topics useful and are very enthusiastic for a follow-up to the workshop which would have more hands-on activities. A number of the participants have even discussed going into collaborative work particularly in the search for bioactive natural products which will be good scaffolds for combinatorial chemistry.

At the last round table discussion, the setting up of a regional network for combinatorial chemistry in Southeast Asia was proposed. This will facilitate regular interactions among the different institutions that will be carrying out CC/CT in the region.

Because most of the objectives of the workshop were met, it is deemed that the workshop has been a success.

Appendix 2. List of Participants

A. Speakers

- Dr. Franciscus Th. M. van Amsterdam
- Dr. Anneliese Appleton
- Dr. Lucia Carrano
- Dr. Giorgio Fassina
- Prof. Stanislav Miertus
- Dr. Pierfausto Seneci

B. International Participants

- Chantana Aromdee, PhD (Thailand)
- Angkana Herunsalee, PhD (Thailand)
- Hai Thanh Ho, PhD (Vietnam)
- Pi Chou Lin, MSc (Taiwan)
- Sree Rama M. Magudula, PhD (India)
- Mohd Ali Mustafa, PhD (Malaysia)
- Suwunna Soontranon, PhD (Thailand)
- Duang Chan Suprasert, PhD (Thailand)
- Po-Keung Wong, PhD (Hongkong) •

C. Local Participants

1. Academe

- Evamarie P. Capareda, PhD
- Christian Joseph Cumagun, MSc
- Ivan Marcelo Duka, MSc
- Ramon S. del Fierro, PhD
- Raymond B. Monterey
- Elmer-Rico E. Mojica
- Jose H. Santos, PhD
- Emma Suplido, MSc

2. Government and Research Institutions

- Sharon Rose García
- · Edwin Alcantara, PhD
- Edna DC Nacianceno

3. Industry

- Danilo Años
- Romulo D. Conde --
- Jose O. Juliano, PhD
- Rosalina D. Nolasco
- Ang Long Bing M. Pao
- George A. Salvilla, MBA
- · Elizabeth T. Tan, PhD

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Appendix 3. Programme

		10 1-	21		
MC	nday, .	-			
	9:00	AM	Opening Ceremonies		40.14
				•	nd B. Monterey
			********		nasco Peñalba
			ICS-UNIDO Programme and Activities		
					ofe A. Calanasan
			Introduction of Participants	Roy Rol	berto L. Gerona
				Emesto	J. del Rosario
	10:00	\mathbf{AM}	COFFEE BREAK		
	11:00	AM	Combinatorial Chemistry and Combinator	orial Te	chnologies: An Overview
			Prof. State	nislav M	Mertus, Dr. Giorgio Fassina
	12:00	NN	Solid Phase Synthesis: An Overview		Dr. Plerfausto Seneci
	12:45	PM	LUNCH		
	2:00	PM	Case Study 1: Solid Phase Synthesis		Dr. Pierfausto Seneci
	2:30	PM	Round Table Discussion on the Morning		
	3:00	PM	Combinatorial Synthetic Libraries: Design		
				,	Dr. Pierfausto Seneci
	4:00	PM	COFFEE BREAK		
	4:30	PM	Solid Phase Synthetic Libraries		Dr. Pierfausto Seneci
	5:30	PM	Case Study 2: Solid Phase Synthetic Lib		
	6:00	PM	Round Table Discussion on the Afternoon		
	••••	• • •	,		
Tu	esday,	20 AD	ril		
	9:00	AM		m Solid	Phase Libraries .
			•		Dr. Pierfausto Seneci
	10:00	AM	Case Study 3: Structure Determination,	/Deconv	volution
			-	,	Dr. Pierfausto Seneci
	10:30	AM	COFFEE BREAK		
	11:00	AM	Solution Phase Synthetic Libraries		Dr. Pierfausto Seneci
	12:00	NN	Case Study 4: Solid Phase Libraries		Dr. Pierfausto Seneci
	12:30	PM	Round Table Discussion on the Morning	Session	n
	1:00	PM	LUNCH		
	2:30	PM	Purification and Quality Control of Librar	ries	Dr. Pierfausto Seneci
	3:30	PM	Solid Phase Oligomeric Synthetic Librari		tides and Nucleotides
				•	Dr. Giorgio Fassina
	4:30	PM	COFFEE BREAK		
	5:00	PM	Case Study 6: Solld Phase Oligomeric Li	ibraries	Dr. Giorgio Fassina
	5:30	PM	Biological Libraries		Dr. Glorgio Fassina
	6:30	PM	Round Table Discussion on the Afternoo	on Sessi	ion
We	ednesda	ay, 21	! Aprîl		
	9:00	AM	Computational Methods in Library Desig	<u>J</u> n	Dr. Anneliese Appleton
	10:00	AM	Softwares for Combinatorial Technologic	es	Dr. Anneliese Appleton
	11:00	AM	COFFEE BREAK		
	11:30	AM	Case Study 7: Computational Methods in	n Librar	y Design
			•		Dr. Anneliese Appleton
	12:00	NN	Round Table Discussion on the Morning		• •
	12:30	PM	LUNCH		
	2:00	PM		Dr. Fran	nciscus van Amsterdam
	3:00	PM	LTS, MTS and HTS: Implications for Dru		
		-			nciscus van Amsterdam
•	4:00	PM	COFFEE BREAK		
	4:30	PM	Case Study 8: Low Throughput Screening	ng <i>Dr</i>	. Franciscus van Amsterdam
	5:00	PM	Case Study 9: High Throughput Screening		. Franciscus van Amsterdam
	5:30	PM	Country Report (Hongkong)		Dr. Po-Keung Wong

	5:45 7:30	PM PM				
Th	ursday	. 22 A	April	•		
	9:00	AM	Natural Products: An Overview	Dr. Lucia Carrano		
	10:00	AM	Natural Products as Sources of Relevant Drug	Natural Products as Sources of Relevant Drugs Dr. Lucia Carrano		
	11:00	AM	COFFEE BREAK			
	11:30	AM	Case Study 10: Natural Products and Drug Di	scovery <i>Dr. Lucia Carrano</i>		
	12:00	NN	LUNCH	•		
	2:00	PM	Case Study 11: Combinatorialization of Natura	al Products		
				Dr. Pierfausto Seneci		
	3:00	PM	Round Table Discussion on Natural Products a	and Combinatorial		
			Technologies			
	3:30	PM	Patenting Issues in Combinatorial Technologic	es <i>Dr. Pierfausto Seneci</i>		
	4:30	PM	COFFEE BREAK			
	5:00	PM	Economics of Combinatorial Chemistry and Te	echnologies		
				Dr. Giorgio Fassina		
	6:00	PM	Round Table Discussion on Patenting Issues a Technologies	and Eonomics of Combinatorial		
Fri	iday, 23	3 Apri	y.			
	8:30	ΑM	Country and Institutional Reports			
	11:00	AM	COFFEE BREAK			
	11:30	AM	Round Table Discussion: Future Actions			
	12:00	NN	Closing Ceremonles			
			Workshop Assessment and Summary	Dr. Pierfausto Seneci .		
				Dr. Cleofe A. Calanasan		
			Response from Participants	Dr. Mohd Ali Mustafa		
				Ms. Rosalina Nolasco		
			BLANCE CONTROL CALLS	Ms. Emma Suplido		
			Distribution of Certificates of Attendance	Prof. Stanislav Miertus		
			Charles Bassada	Ms Betty Koreh		
	1,00	DAA	Closing Remarks	Dr. Norma N. Fajardo		
	1:00	PM	END OF WORKSHOP LUNCH			

Appendix 4. Summary of the Questionnaire Results

A. Organization

	Excellent	Very Good	Good	Fair
Information Process	41%	35%	24%	0%
Announcement and Pre-course material	25%	31%	31%	13%
Scientific Programme	41%	59%	0%	0%
Applied Lecture/Workshop	25%	69%	6%	0%
Small working groups	25%	50%	25%	0%
Case Studies	35%	53%	12%	0%
Question Time	35%	41%	24%	0%

	Balanced	Not Balanced
Participants' Scientific Knowledge	79%	21%

B. Duration of Programme

	Just Right	Too Long	Too Short
Number of Days	94%	6%	0%
Length of Working Days	71%	29%	0%

C. Training Facilities and Hotel

	Excellent	Very Good	Good	Fair
Lecture/Training Rooms	47%	41%	12%	0%
Breaks/Refreshments	65%	29%	6%	0%
Hotel Accommodation	29%	36%	29%	7%
Meals at Hotel	64%	14%	22%	0%

D. Organizer's Response to Participants' needs

	Excellent	Very Good	Good	Fair
Г	65%	24%	11%	0%

E. Overall programme organization

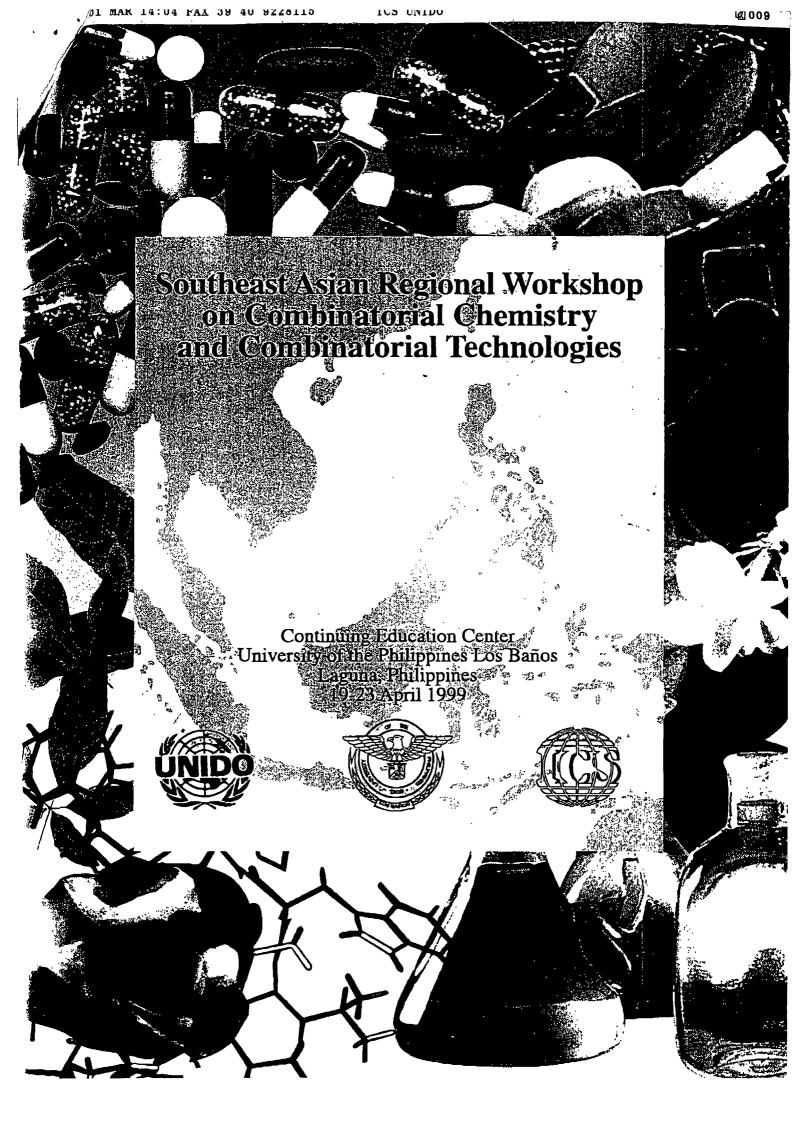
Excellent	Very Good	Good	Fair
59%	41%	0%	0%

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

	Yes	Maybe	No
Γ	100%	0%	0%

G. Evaluation of Lecturers and Speakers

	Excellent	Very Good	Good	Fair
Course Materials	38%	56%	6%	0%
Resident Lecture presentation	44%	56%	0%	0%
International Presentation	50%	44%	6%	0%
Ability to Answer Specific Questions	44%	56%	0%	0%



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